Simulation-Enabled Discoveries: Examples from MHD and Turbulence

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Discovery through simulation

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AMS Seminar Series

NASA Ames Research Center

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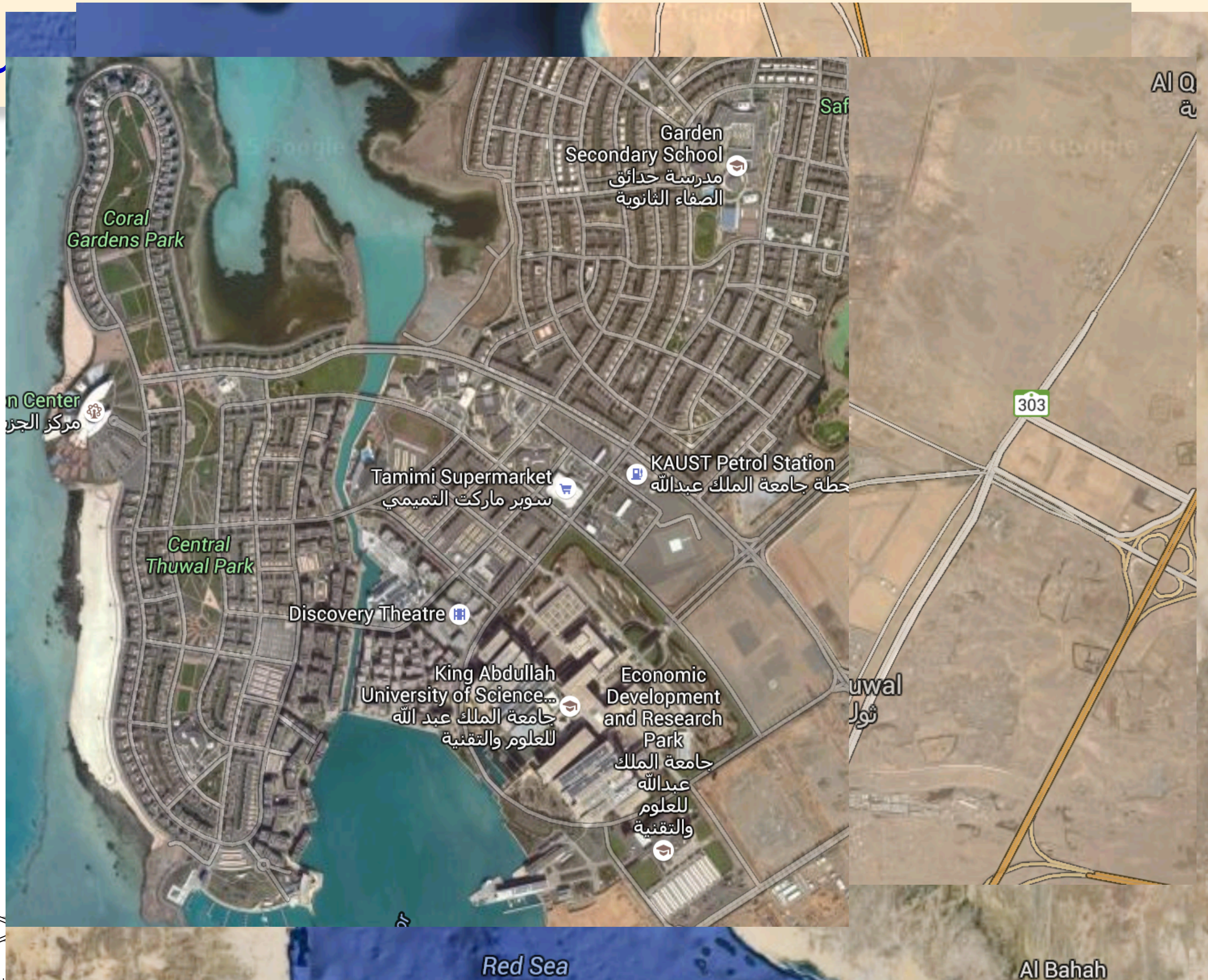

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Research Philosophy

- Classical example of simulation enabled discovery
  - *Discovery of the soliton by Martin Kruskal and Norman Zabusky (Phys. Rev. Letters 1965)*
- "Our present analytical methods seem unsuitable for the solution of the important problems arising in connection with nonlinear partial differential equations and, in fact, with virtually all types of nonlinear problems in pure mathematics. The truth of this statement **is particularly striking in the field of fluid dynamics**…. We conclude by remarking that high speed computing devices … should ultimately lead to important analytical advances" - J. Von Neumann, 1946

- Motto: "**Discovery through simulation**"

- Investigate, through computational and analytical techniques, *clearly posed scientific questions* in physics of fluids/plasmas
  - *Solve interesting and intellectually challenging puzzles*

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Simulation-Enabled Discoveries

- What is a "Discovery"?
  - *Scientific discovery is the process or product of successful scientific inquiry. Objects of discovery can be things, events, processes, causes, and properties as well as theories and hypotheses and their features (their explanatory power, for example).*

    -Stanford Encyclopedia of Philosophy

- What is "Scientific Inquiry"?
  - *Scientific inquiry generally aims to obtain knowledge in the form of testable explanations that can be used to predict the results of future experiments*
  - *The most successful explanations, which explain and make accurate predictions in a wide range of circumstances, are often called Scientific Theories*

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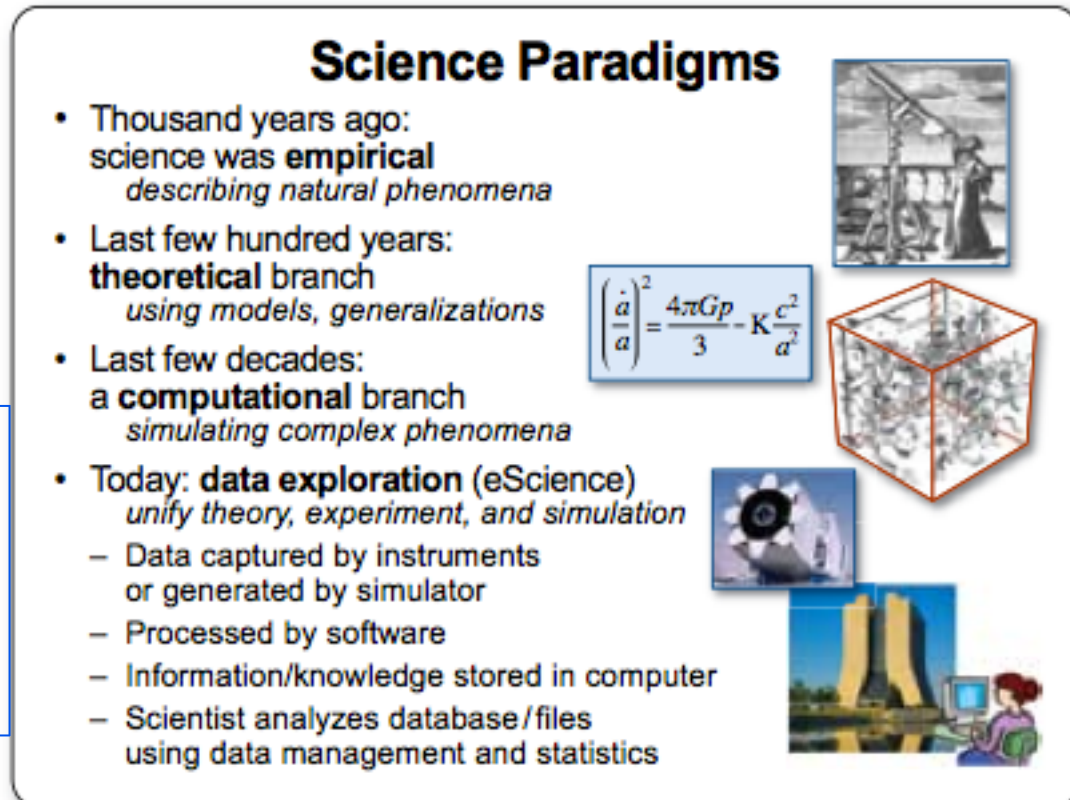
Scientific Inquiry Paradigms

- Experiment/Observation (Empiricism)
- Theory
- Computations (or Simulations)
- Fourth Paradigm: The fourth paradigm for science is one based on data intensive computing



Slide from
Jim Gray, “eScience:
A Transformed
Scientific Method”
in “The Fourth Paradigm”
Edited by Hey et al. 2009

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Scientific Discovery – Some Thoughts

- Discovery
  - *Planned confirmation of hypotheses*
  - *Serendipitous (e.g. Penzias/Wilson cosmic microwave background)*

- Should we consider Higgs Boson or Quarks as "discoveries" until these are confirmed by experimental/observational validation?
  - *No (the Nobel committee believes this)*
  - *Yes, Maybe*

- Likewise, discoveries via simulations should be validated against experiment/observation
  - *Generally, simulations solve some version of "nature's laws" expressed mathematically*
  - *So, in general, it is reasonable to consider that solutions (at least the stable ones) will likely occur in carefully designed experiments if not in nature*
  - *So simulation discoveries are "weak discoveries" –not complete unless validated*

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Scientific Examples (Puzzles)

- MHD: Richtmyer-Meshkov Instability
- MHD: Magnetic Reconnection
- Turbulence: Wall-bounded Turbulence

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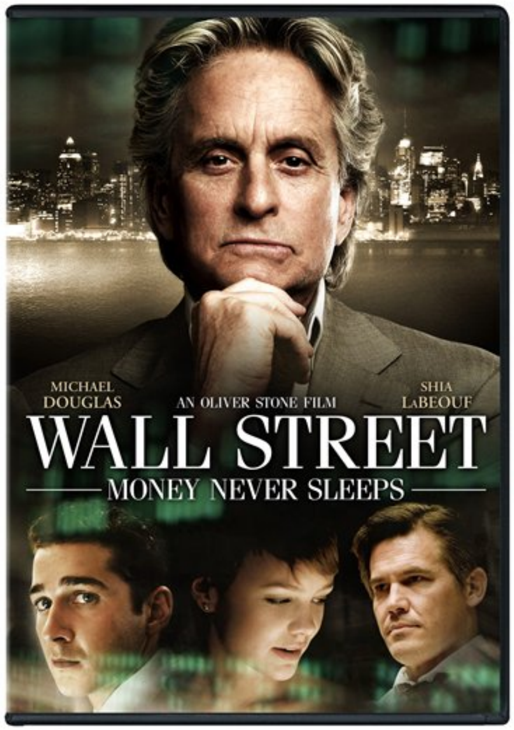
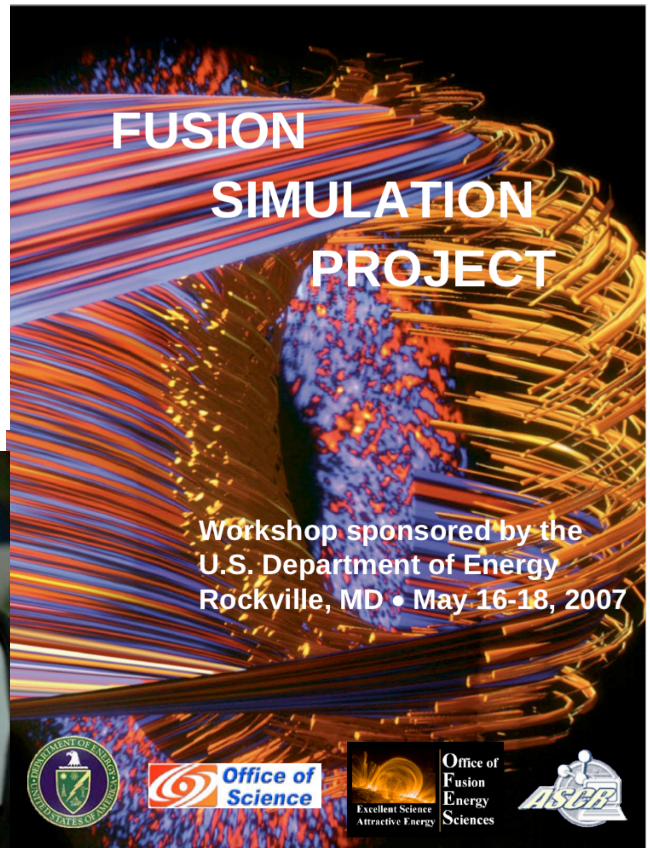
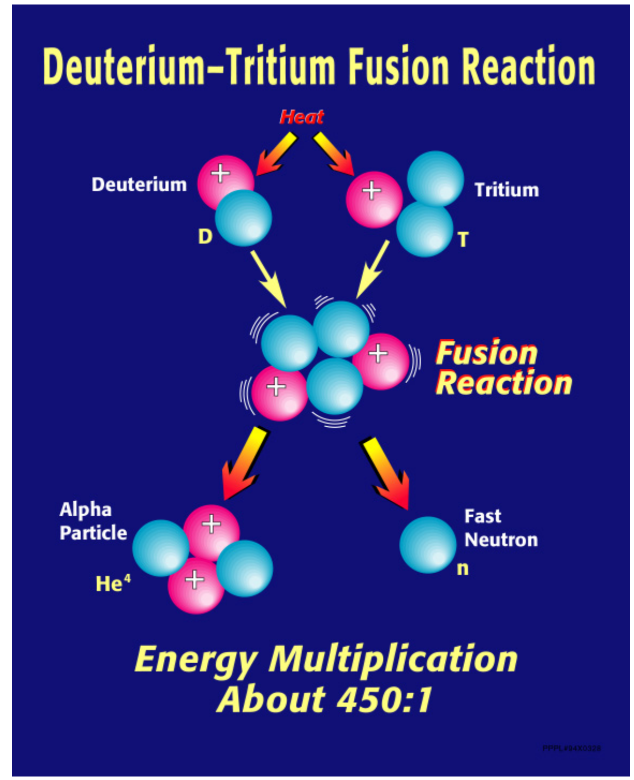
Seen Wall Street 2?   Fusion Energy!



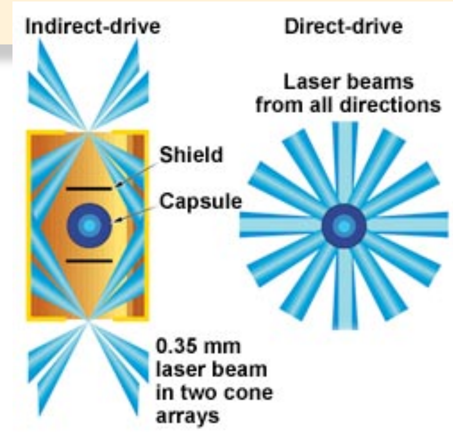




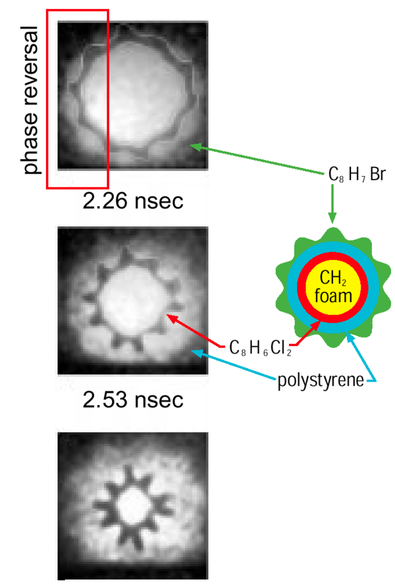
Most "sighted" work

Inertial Confinement Fusion

- National Ignition Facility at LLNL
  - *192 Laser Beams (~500 TW)*
  - *Deposit 1.8 MJ of energy on a hollow gold chamber (Hohlraum)*
  - *Science at the extreme for astrophysics*
- National Ignition Campaign (2009-2012)
  - *No ignition achieved*
- Lindl *et al*. (2014): a comprehensive review of the NIC. In the final section entitled "The Path Forward", the authors write: "*Current evidence points to low-mode asymmetry and hydrodynamic instability as key areas of research to improve the performance of ignition experiments on the NIF and are a central focus of the Ignition Program going forward.*"
- **A key bottleneck towards achieving fusion is hydrodynamic instabilities**



Source: LLNL Website



X-ray images from Nova laser expts. Barnes et al. (1997)

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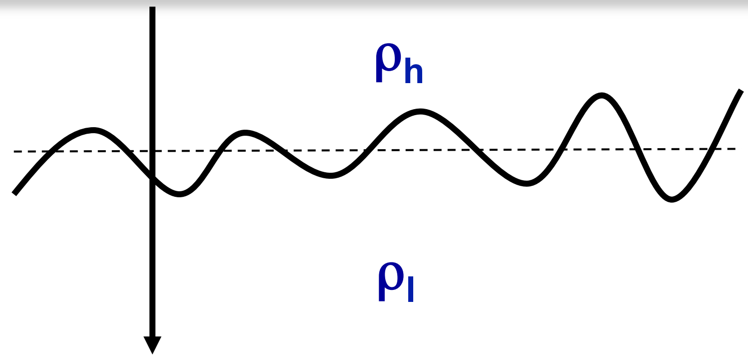
Richtmyer-Meshkov Instability (RMI)

- RMI
  - *occurs at a fluid interface accelerated by a shock-wave*
  - *“impulsive Rayleigh-Taylor”*
  - *Linear stability analysis by Richtmyer (1960)*
  - *Experimental confirmation by Meshkov (1970)*



g(t) = constant (RT)

= Δ U δ (t) (RM)

Growth rate of perturbation:

Exponential (RT)

Linear (RM)

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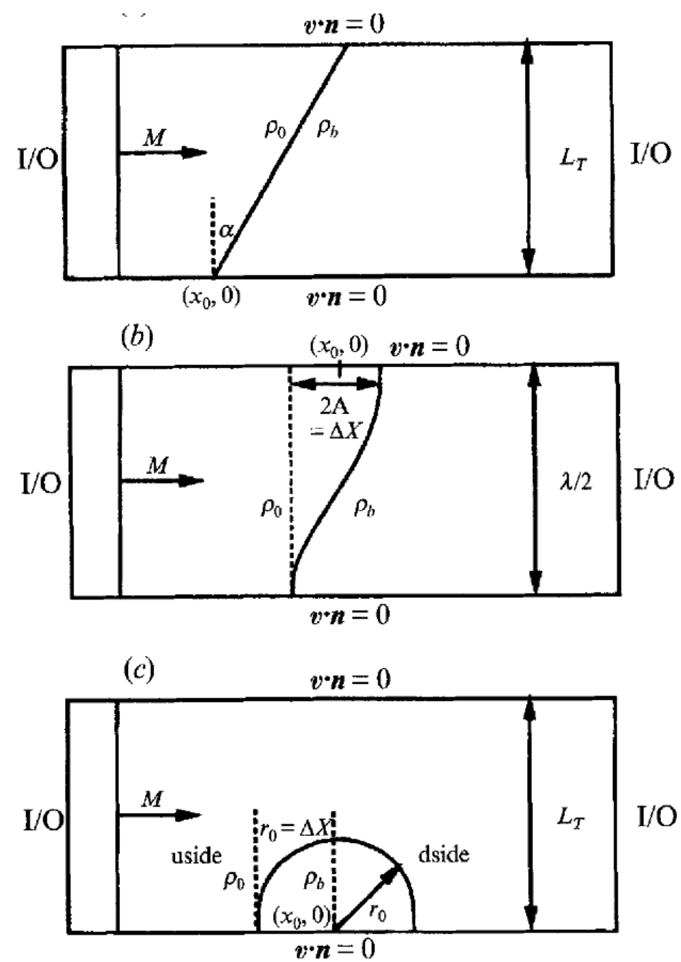
RMI: Configurations and Parameters

- Sawtooth interface (top)
- Single mode interface (middle)
  - *Linear stability*
- Multimode interface (not shown)
  - *Mixing*
- Shock-bubble interactions (bottom)

- Parameters
  - *Mach number of the incident shock, **M***
  - *Density ratio (or Atwood number at the fluid interface), η, **At=(η-1)/(η+1)***
  - *Geometry: Perturbation etc.*
  - *Magnetic field strength $\beta^{-1}=B_0^2/2p_0$*



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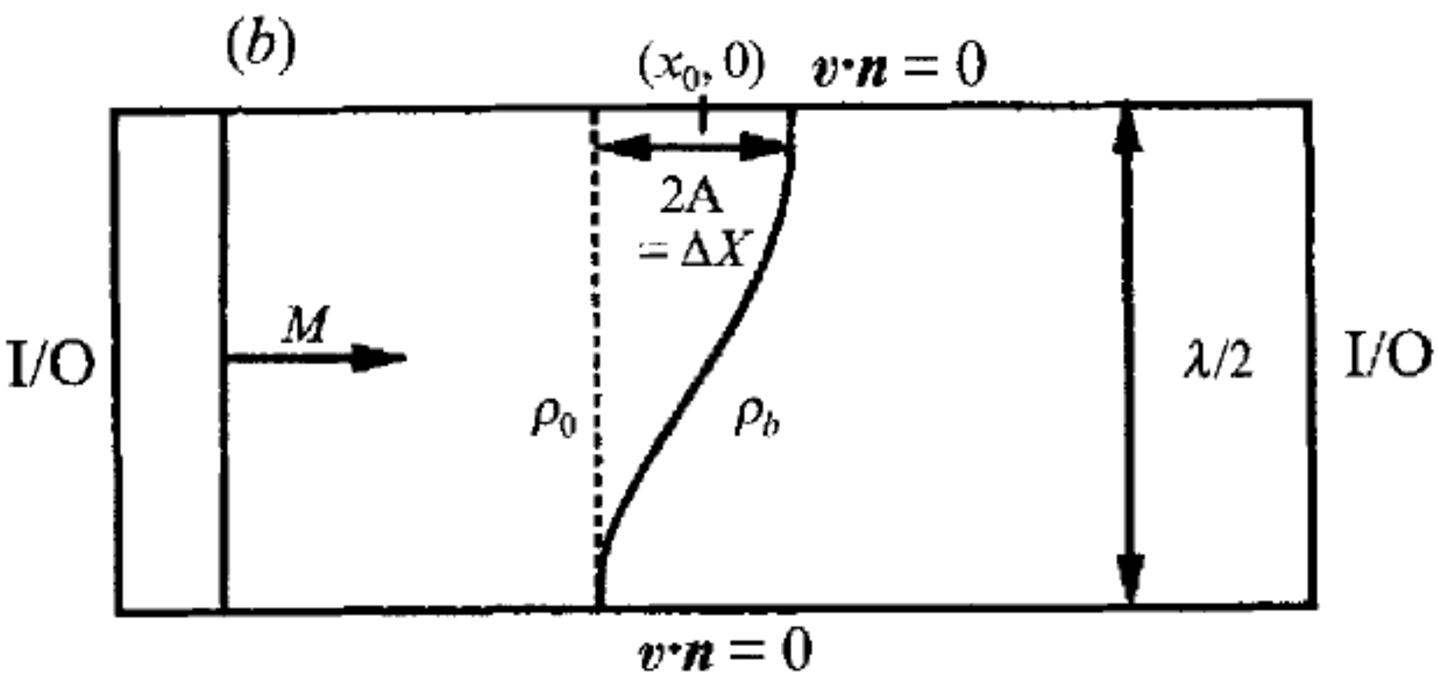
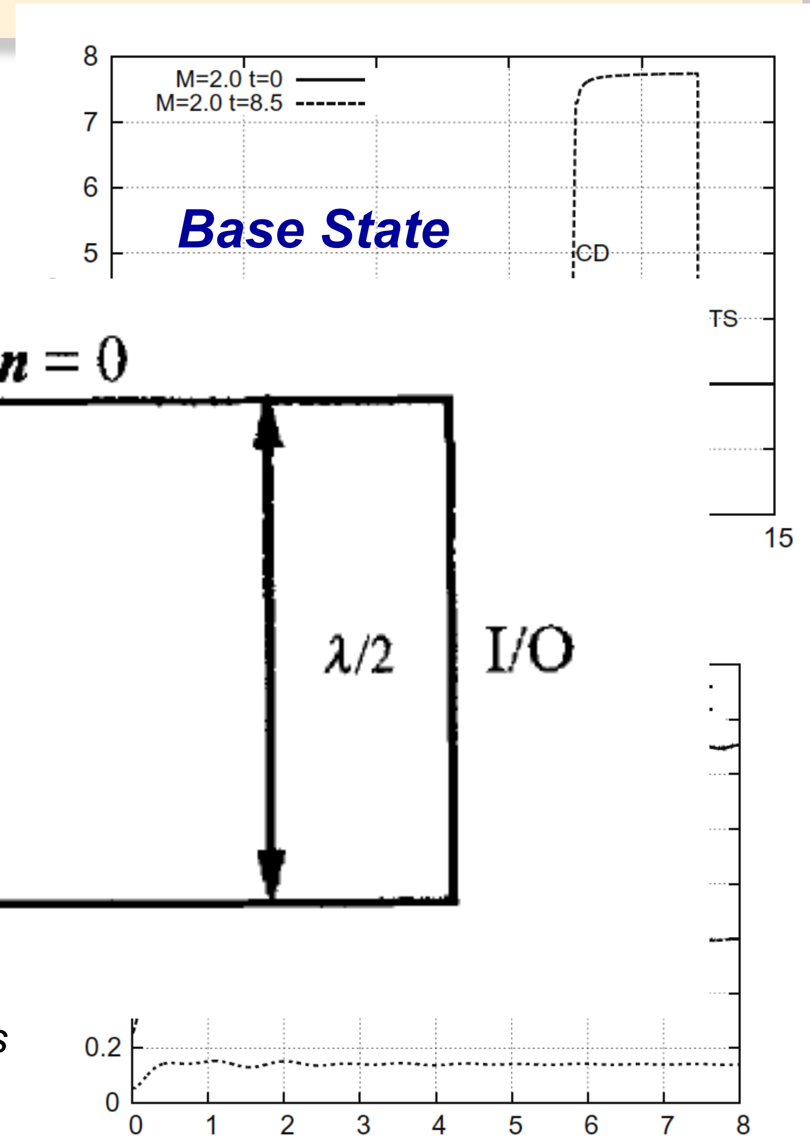
RMI: Linear Stability

- Original theory and numerical simulations by Richtmyer (1960)



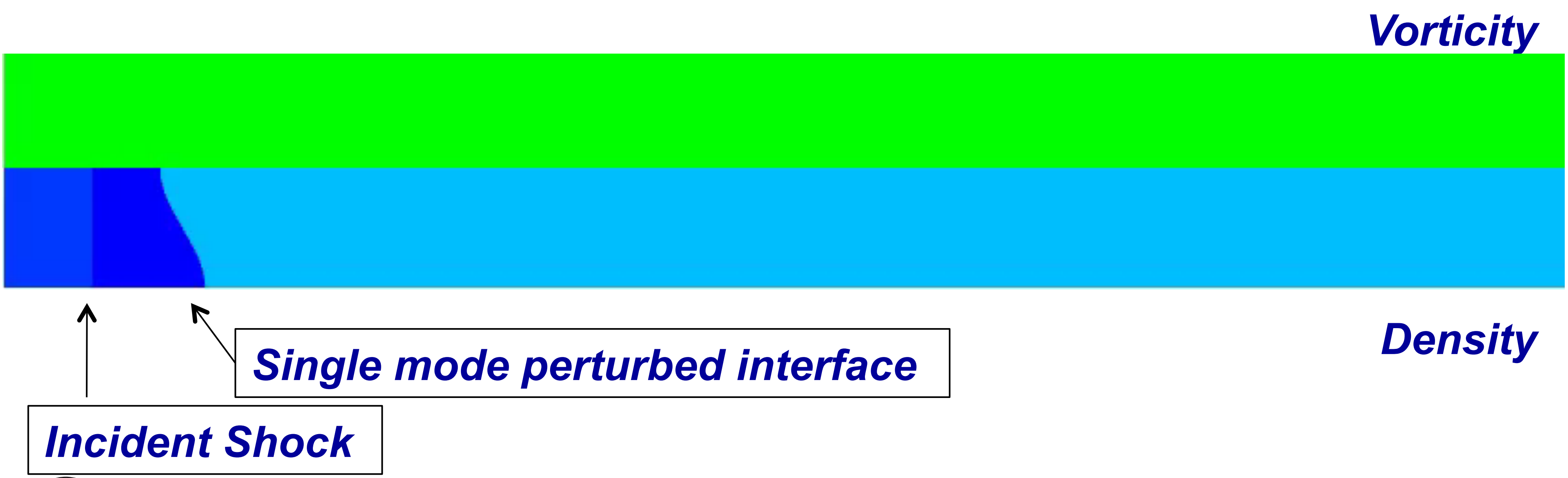


  - *Shock – gas-curtain interactions and others*
- Experimental confirmation by Meshkov (1969)

Figures from Samtaney, JCP 2009

RMI: Single-Mode Interface

- Vorticity generated by baroclinic mechanism
  - *Vortex layer rolls up to a vortex pair*



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Vortex Dynamical Interpretation

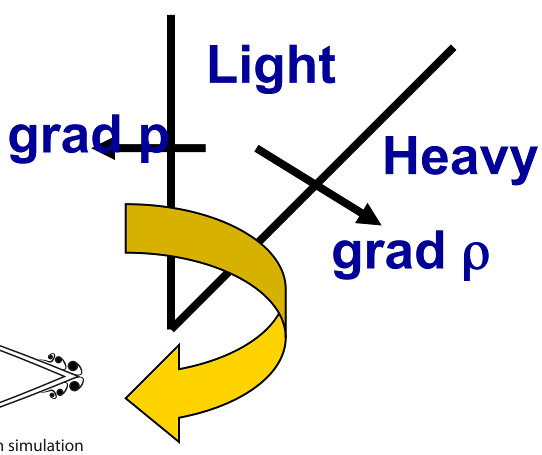
- During incident shock refraction on the density interface vorticity is generated due to misalignment of density and pressure gradients (Hawley and Zabusky, PRL 1989)

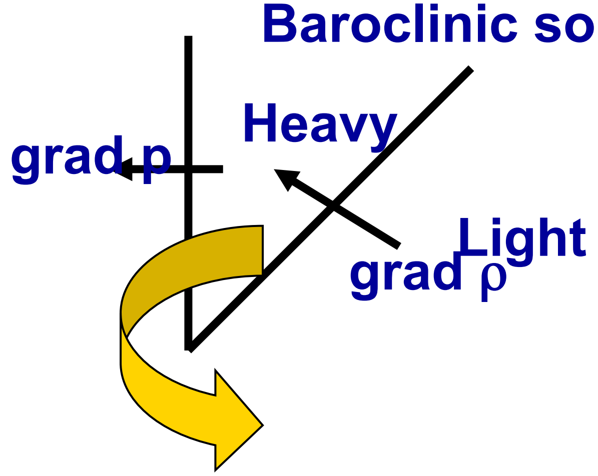
$$\frac{\partial \omega}{\partial t} + (\mathbf{u}\cdot\nabla)\omega = -\omega(\nabla\cdot\mathbf{u}) + \underbrace{\boxed{(\omega\cdot\nabla)\mathbf{u}}}_{=0 \text{ in 2D}} + \underbrace{\boxed{\frac{\nabla\rho\times\nabla p}{\rho^2}}}_{\text{Baroclinic source}} + \underbrace{\boxed{\nabla\times(\rho^{-1}\nabla\times\mathbf{B}\times\mathbf{B})}}_{\text{zero during incident shock refraction phase}}$$

=0 in 2D

zero during incident shock refraction phase

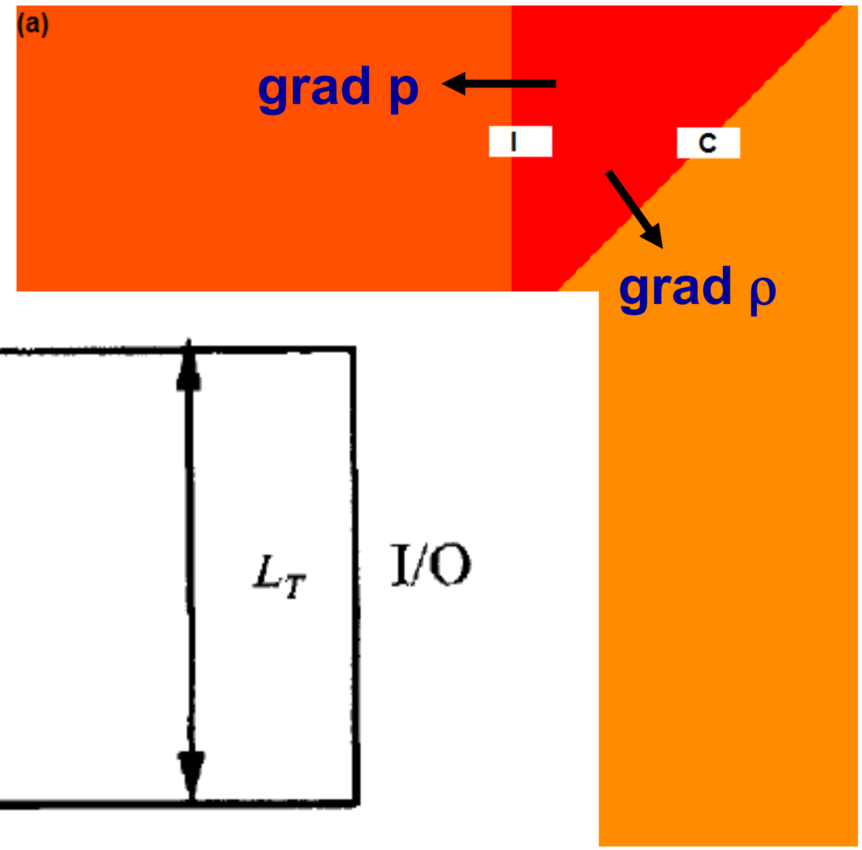
Baroclinic source

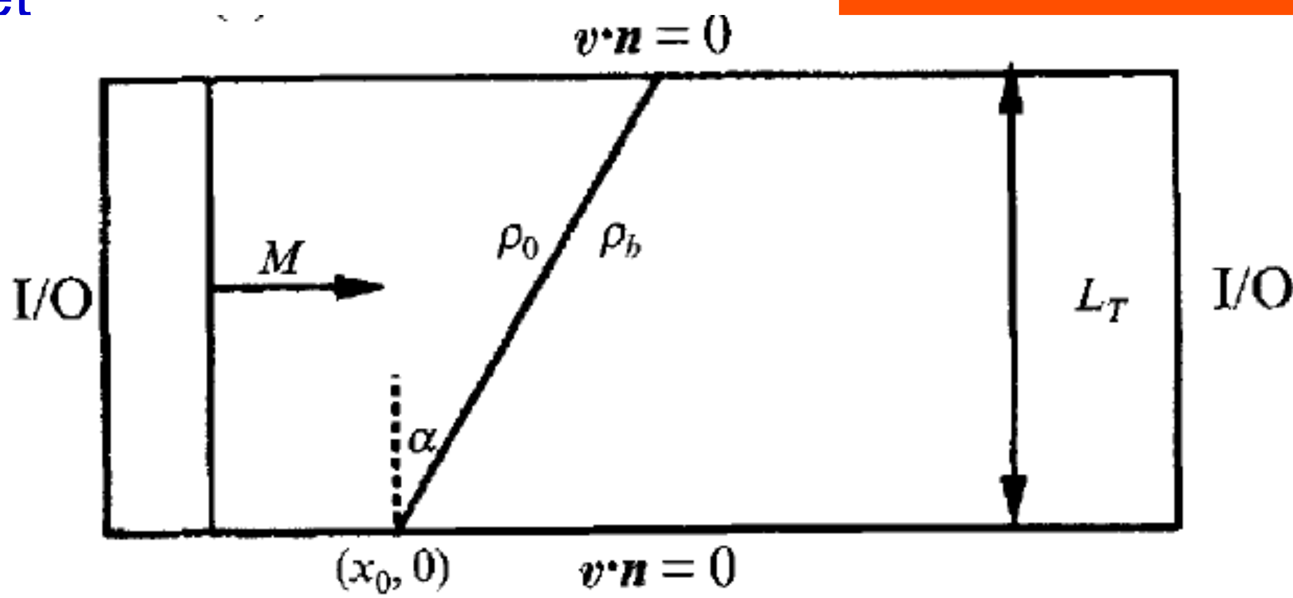




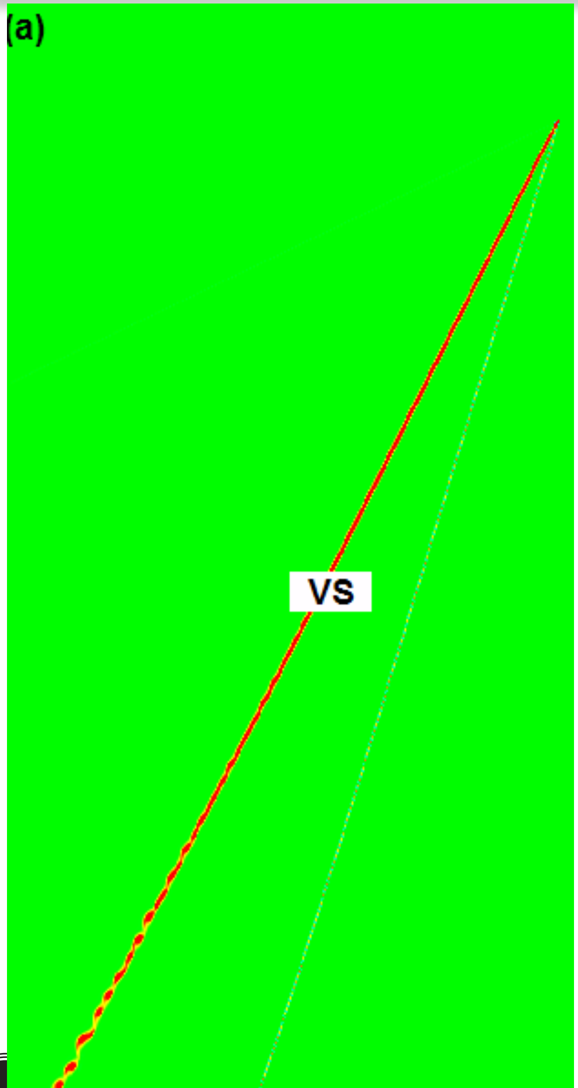
Early Phase – Shock Refraction

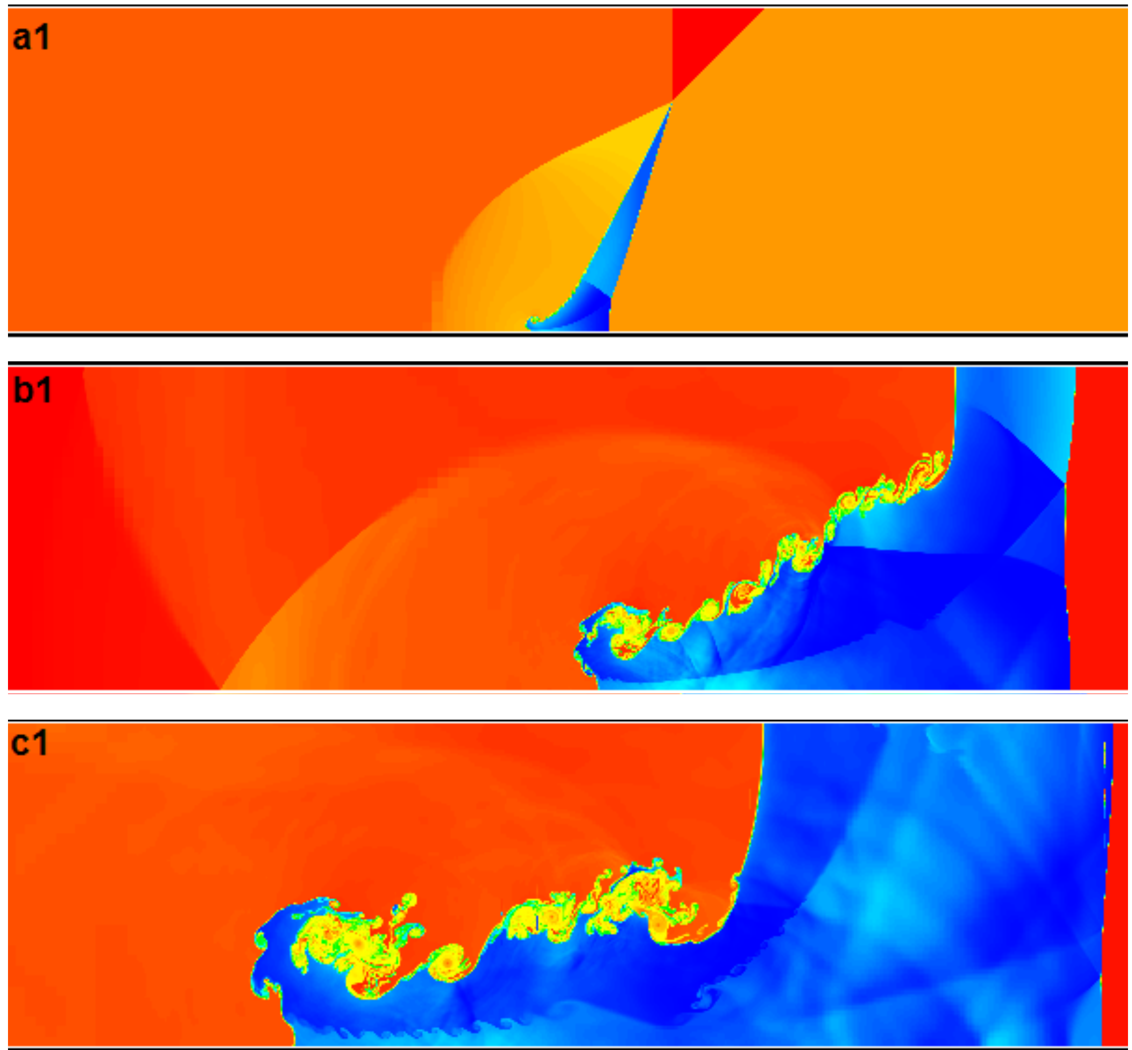
- Incident shock refracts at the interface (contact discontinuity)
  - *Rich set of refraction patterns*
- The shocked contact is a vortex sheet





Vortex Dynamical Interpretation





- Vortex sheet rolls up and interface amplitude increases

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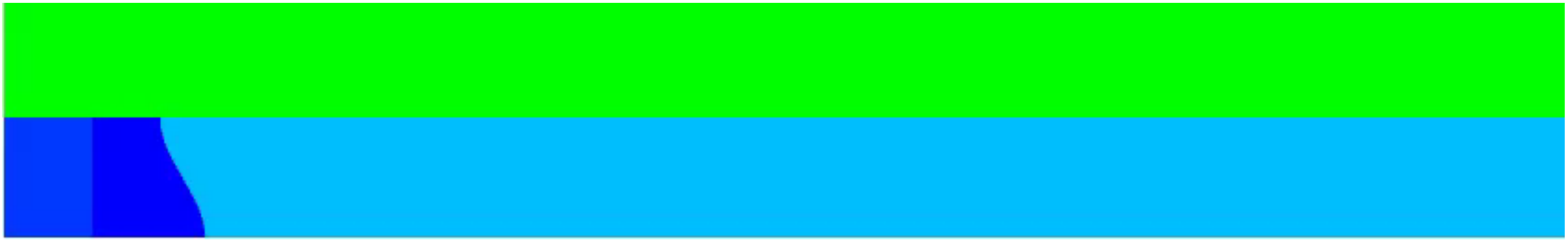
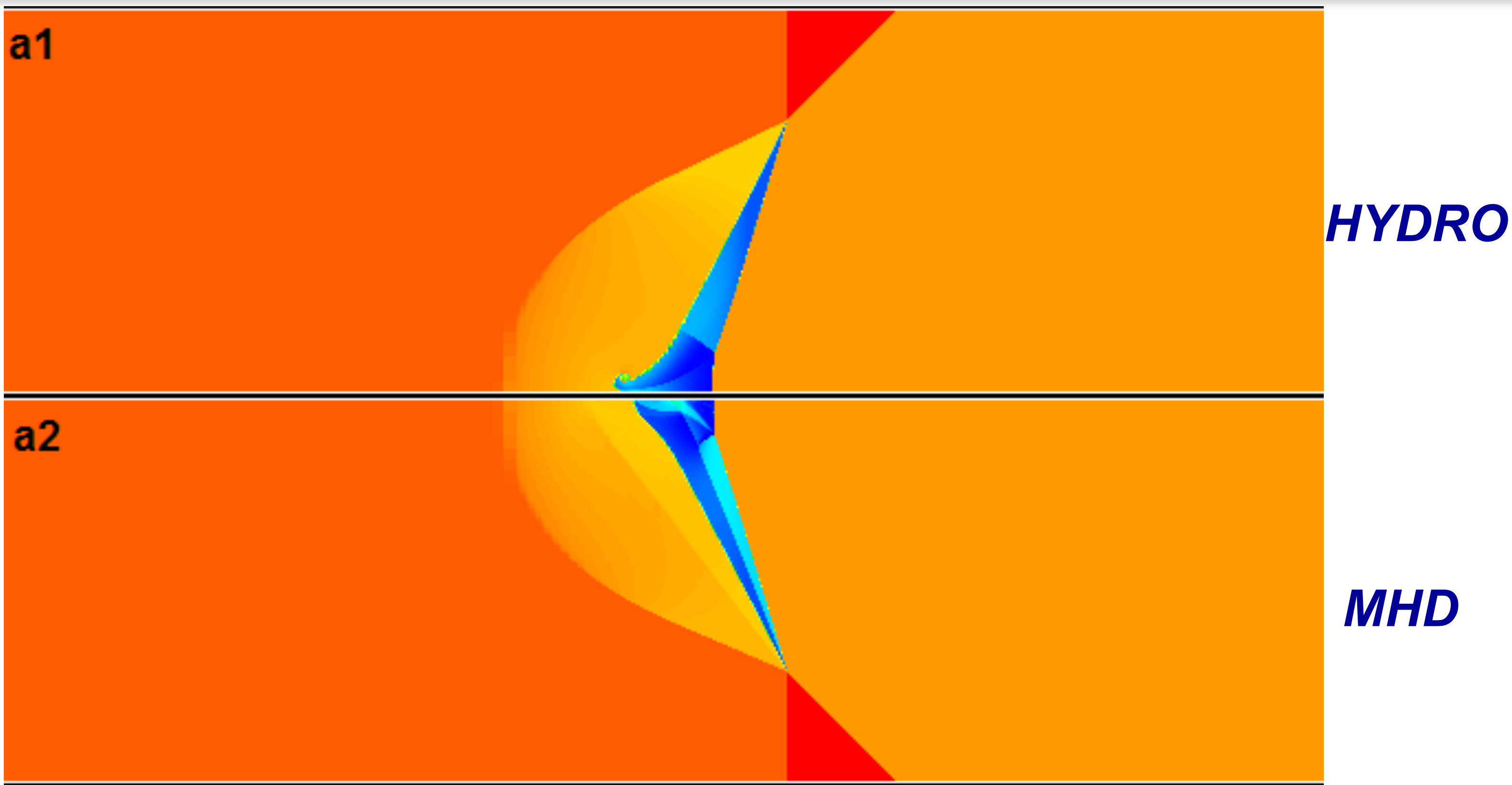
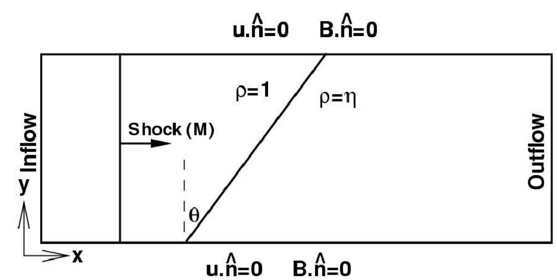
RMI: What happens in the presence of a magnetic field?



RMI: Hydro vs. MHD





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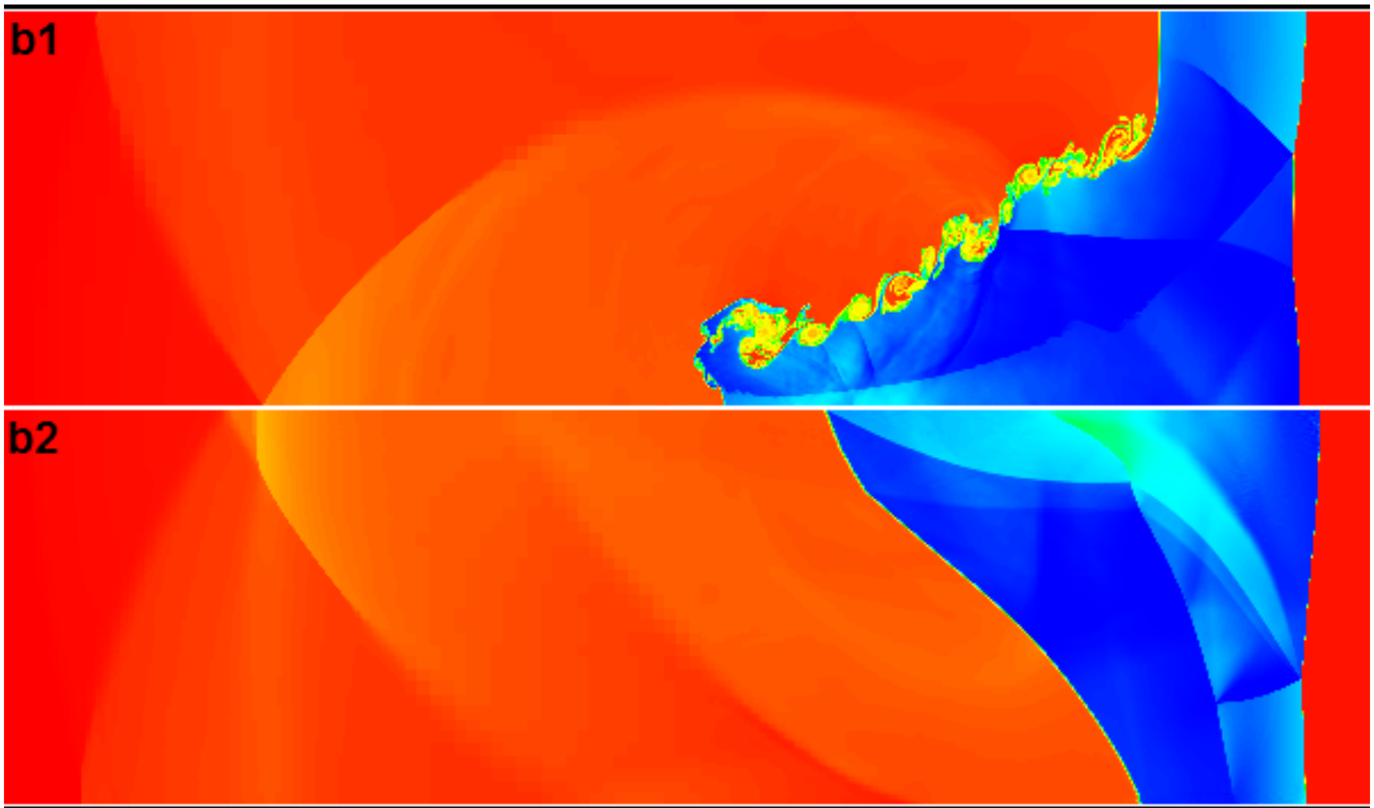
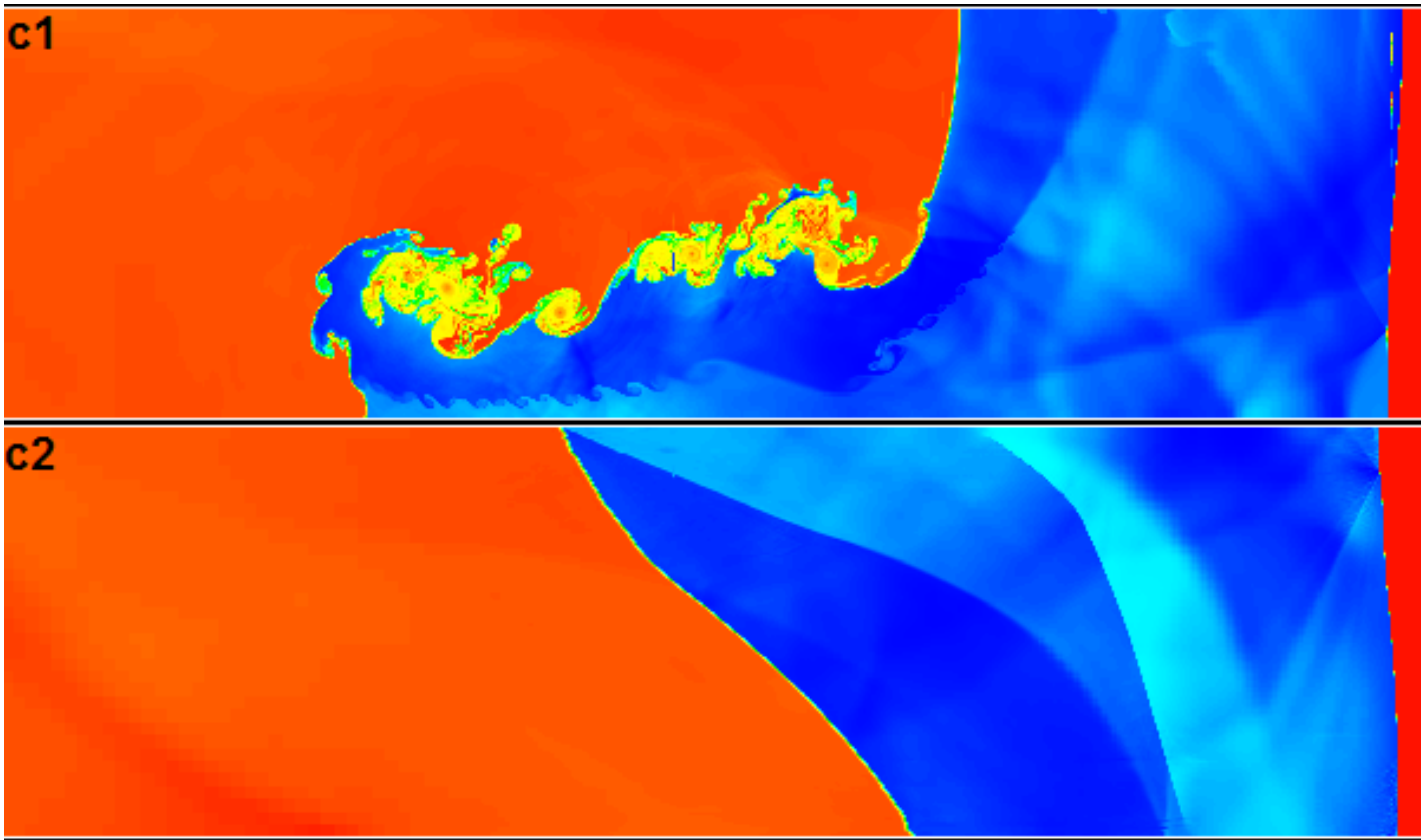
RMI Suppression in MHD

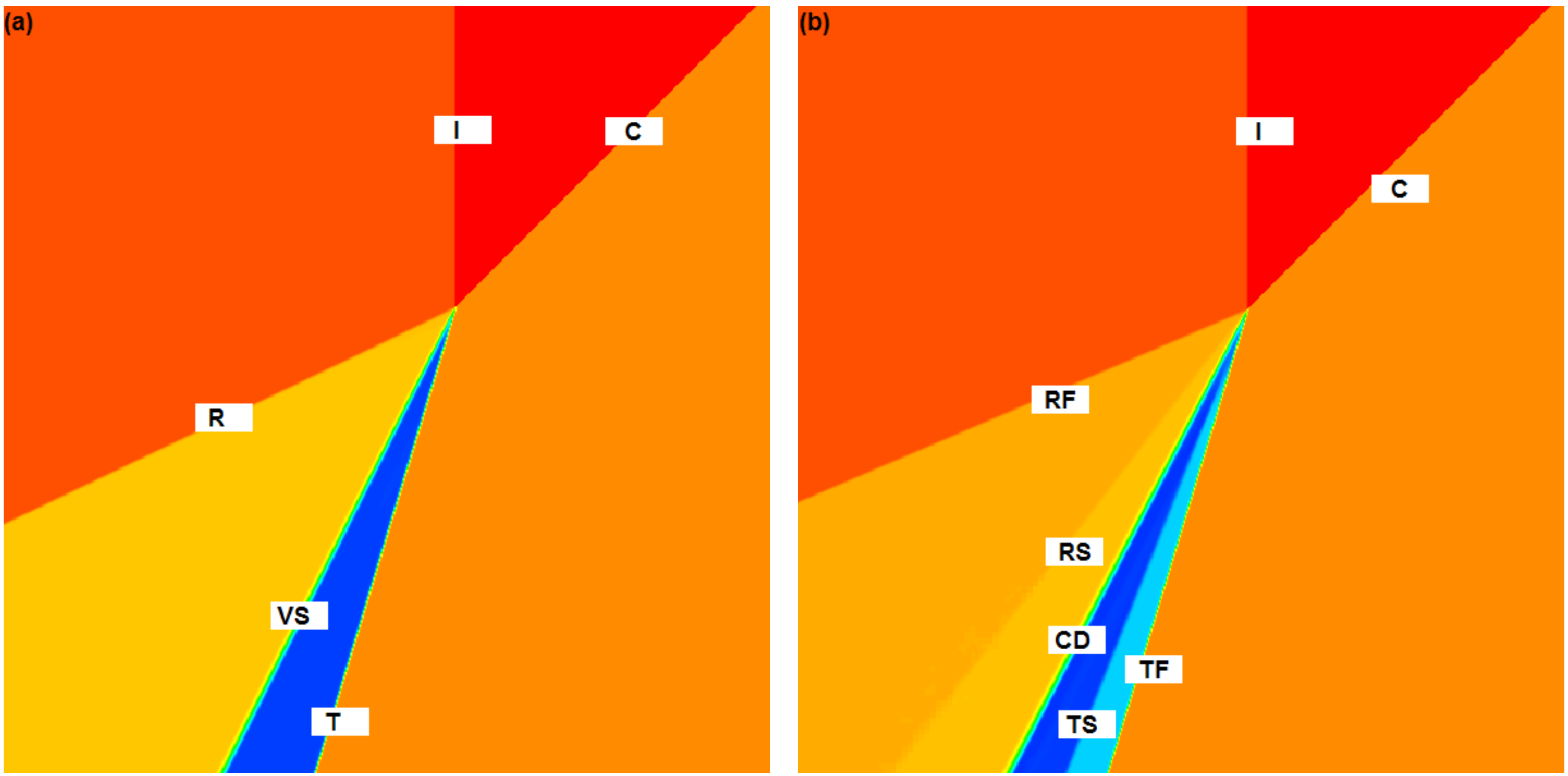


- t=1.86

RMI – Suppression in MHD

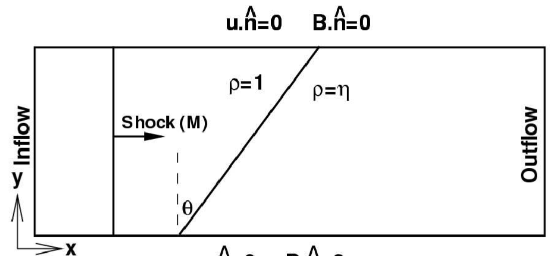


Early Refraction Phase



HYDRO

MHD



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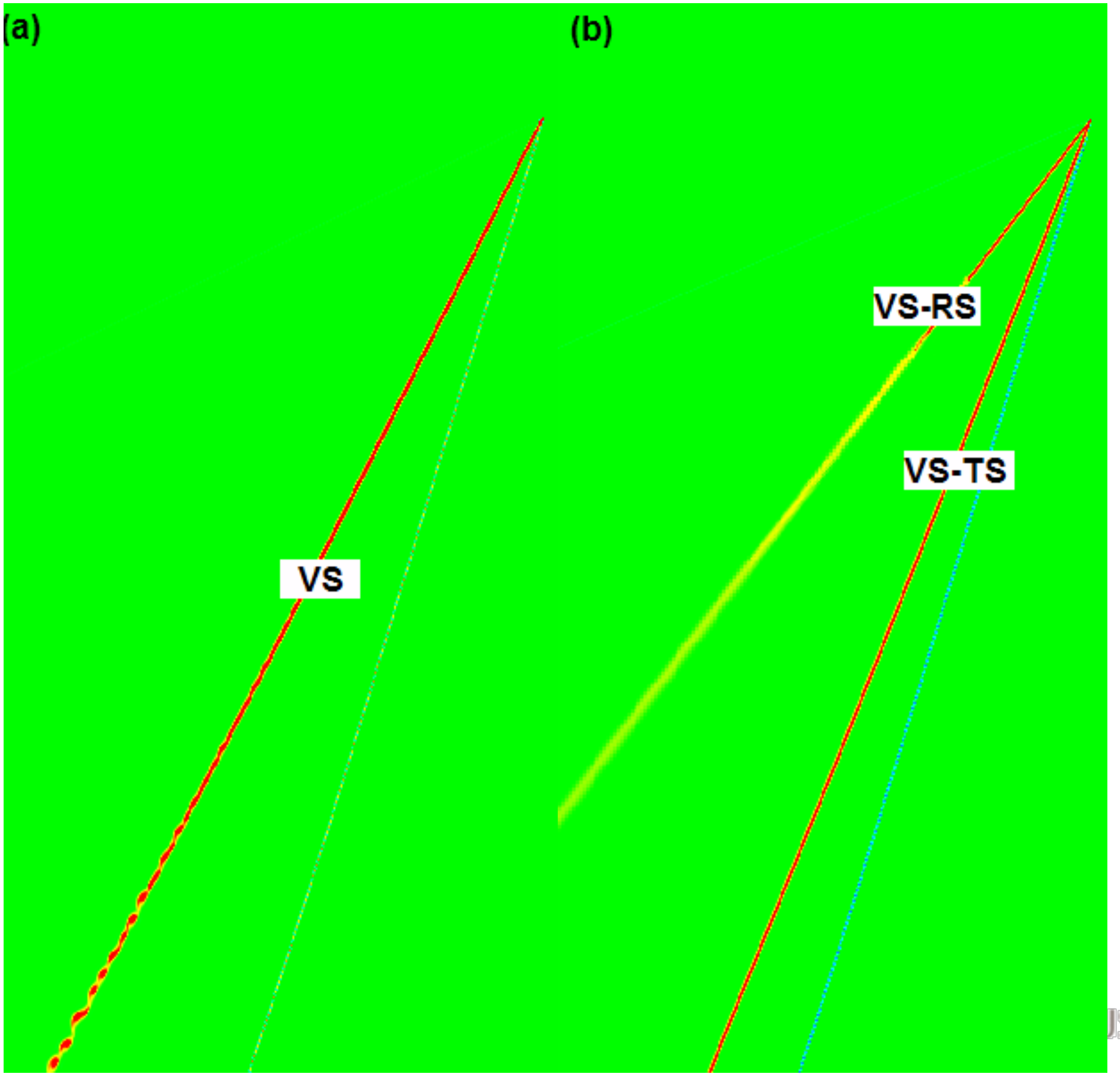
Vortex sheets – Early Refraction Phase

- The shocked interface is a vortex sheet ($\beta^{-1}=0$)
- In MHD shocks can support shear
- MHD→Hydro limit as $\beta^{-1}\rightarrow 0$ is singular (Wheatley et al. JFM 2005)



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MHD Shock Refraction: Local Analysis

- For regular refraction at the contact discontinuity, in a small neighborhood of the point where all discontinuities meet, the MHD PDEs can be reduced to algebraic equations
- TF and RF are fast shocks
- Local analysis shows that the RS is a slow shock, while shock TS is a 2-4 intermediate shock

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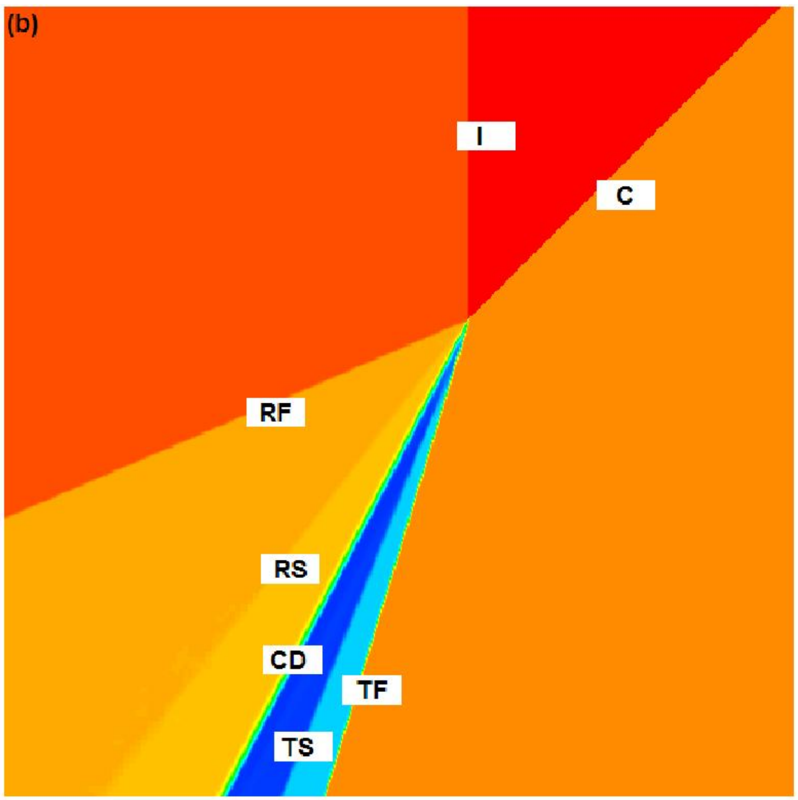
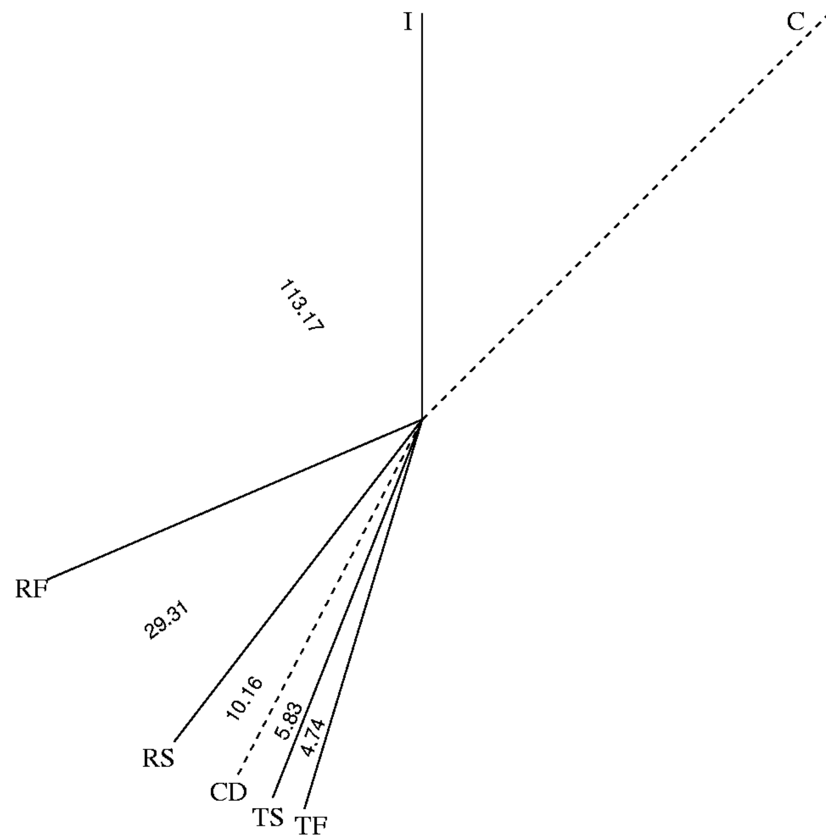
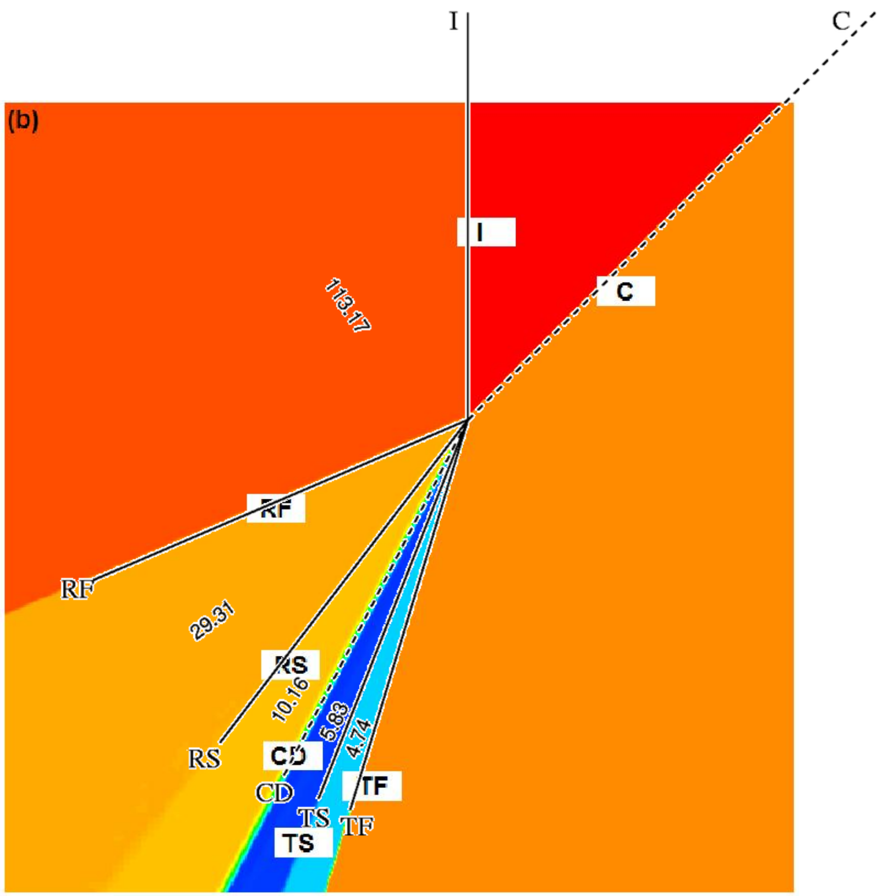
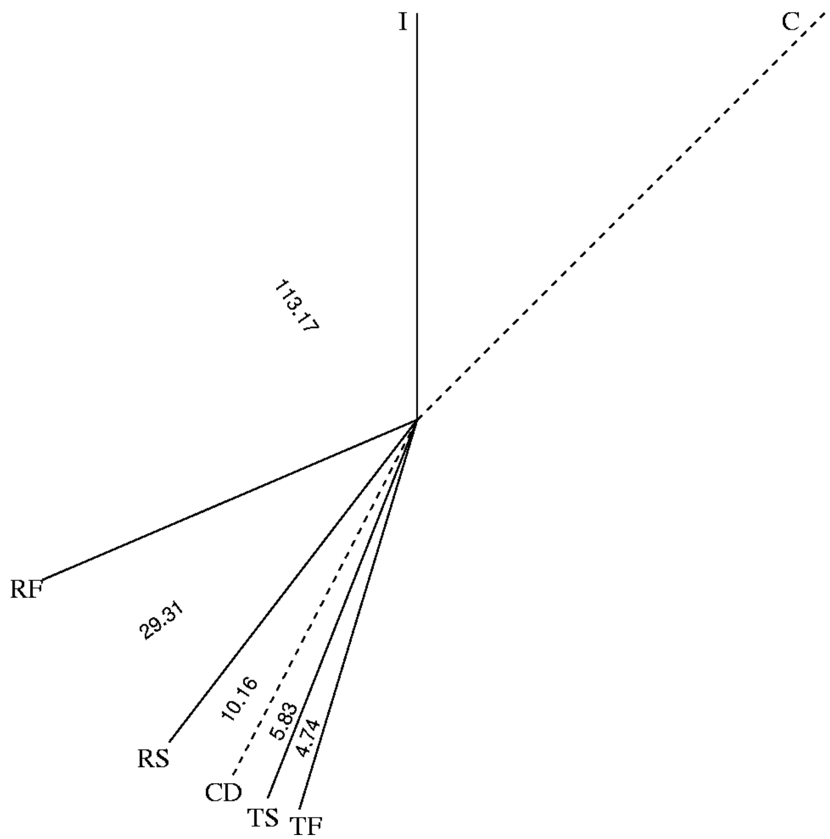
Comparison between Simulation and Local Analysis





Comparison between Simulation and Local Analysis





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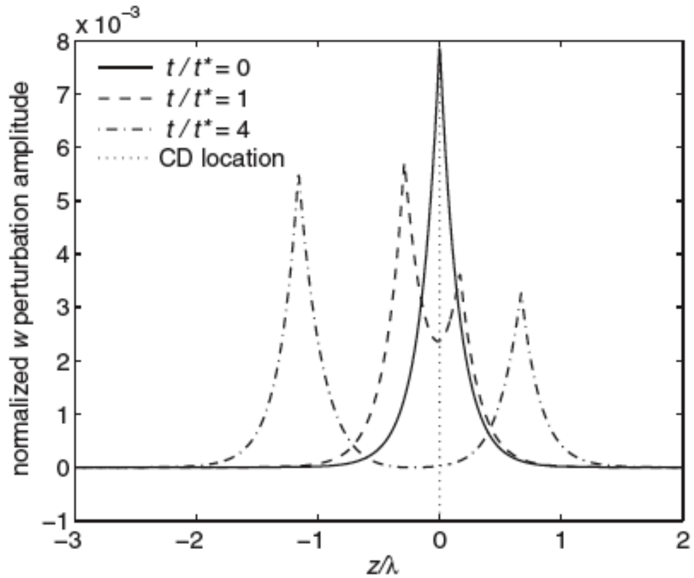
RMI: Linear Stability Analysis in MHD

- Analytical incompressible linear stability theory (Wheatley et al. PRL 2005)
  - At t=0+ we recover the hydrodynamic limit

$$\left.\frac{\partial \eta}{\partial t}\right|_{t=0^+} = \eta_0 k V \mathcal{A},$$



  - Amplitude perturbation grows initially and then saturates at a value given by

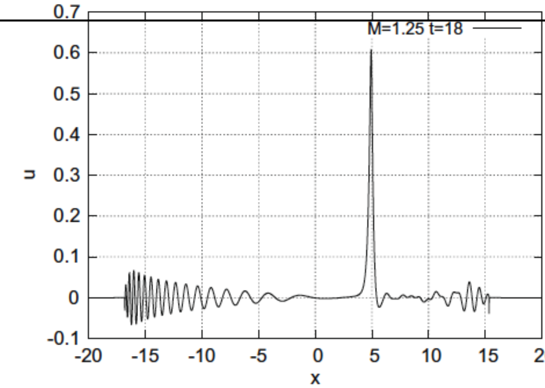
$$\eta_\infty = \eta_0 \left(1 + \frac{\Delta V \sqrt{\mu_0 \rho_1 \rho_2}}{B} \frac{\rho_2 - \rho_1}{\sqrt{\rho_1}\rho_2 + \sqrt{\rho_2}\rho_1}\right)$$

- Two fronts that propagate the local Alfvén speed arise naturally in the solution.

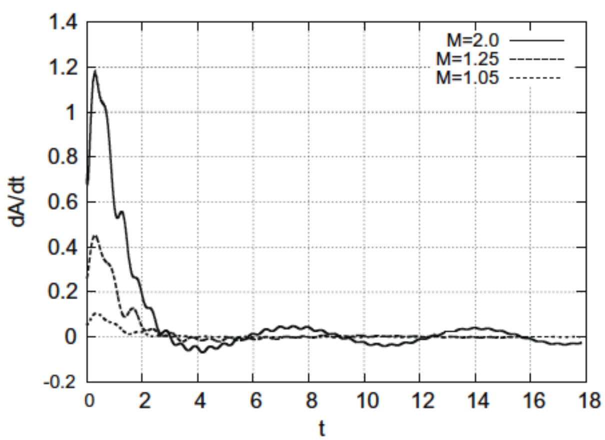
RMI: Linear Compressible MHD

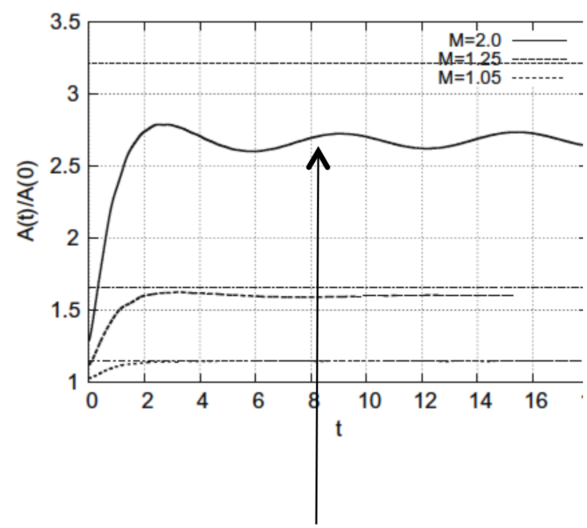
- Linearized compressible MHD solution obtained numerically

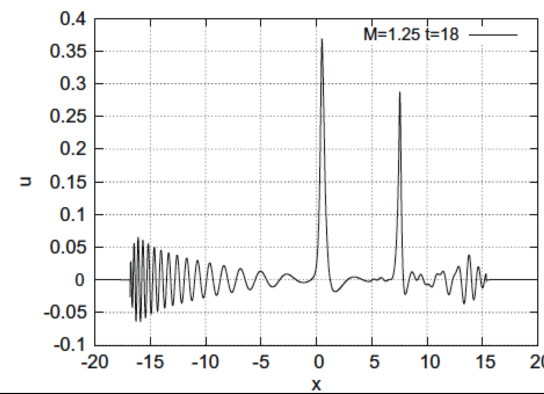
Hydro: Vorticity remains on the interface



(a)







(c)

MHD: Growth rate decays to zero and amplitude saturates

MHD: Vorticity taken away by Alfvén fronts

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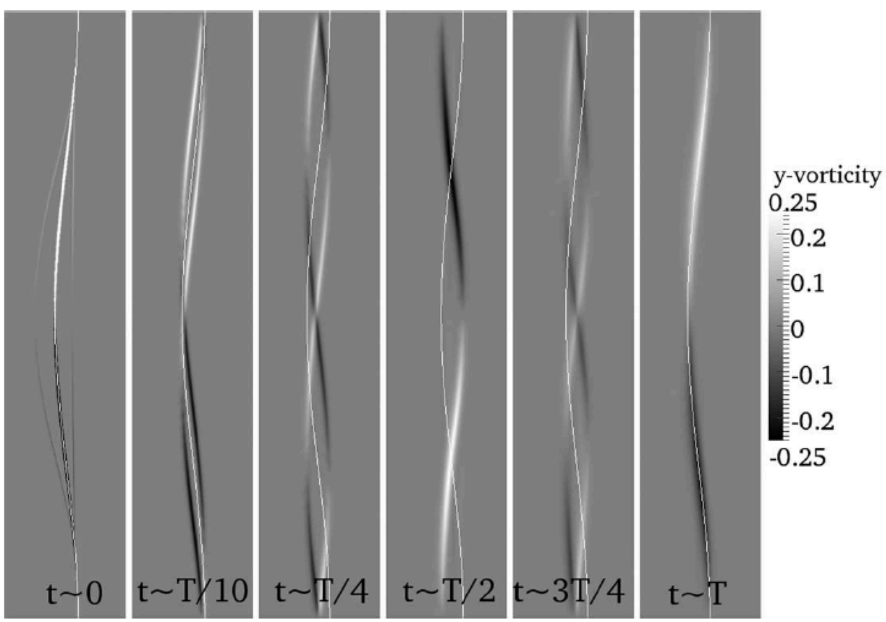
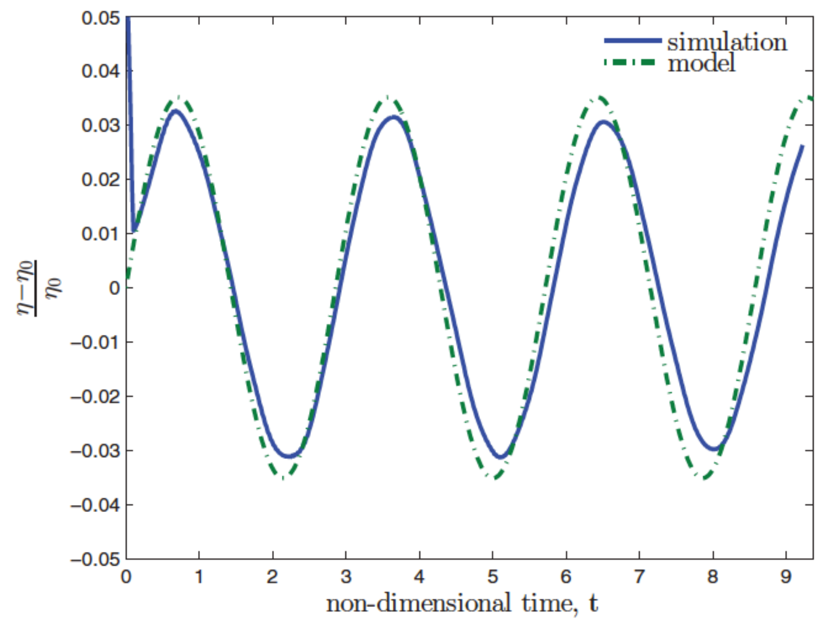
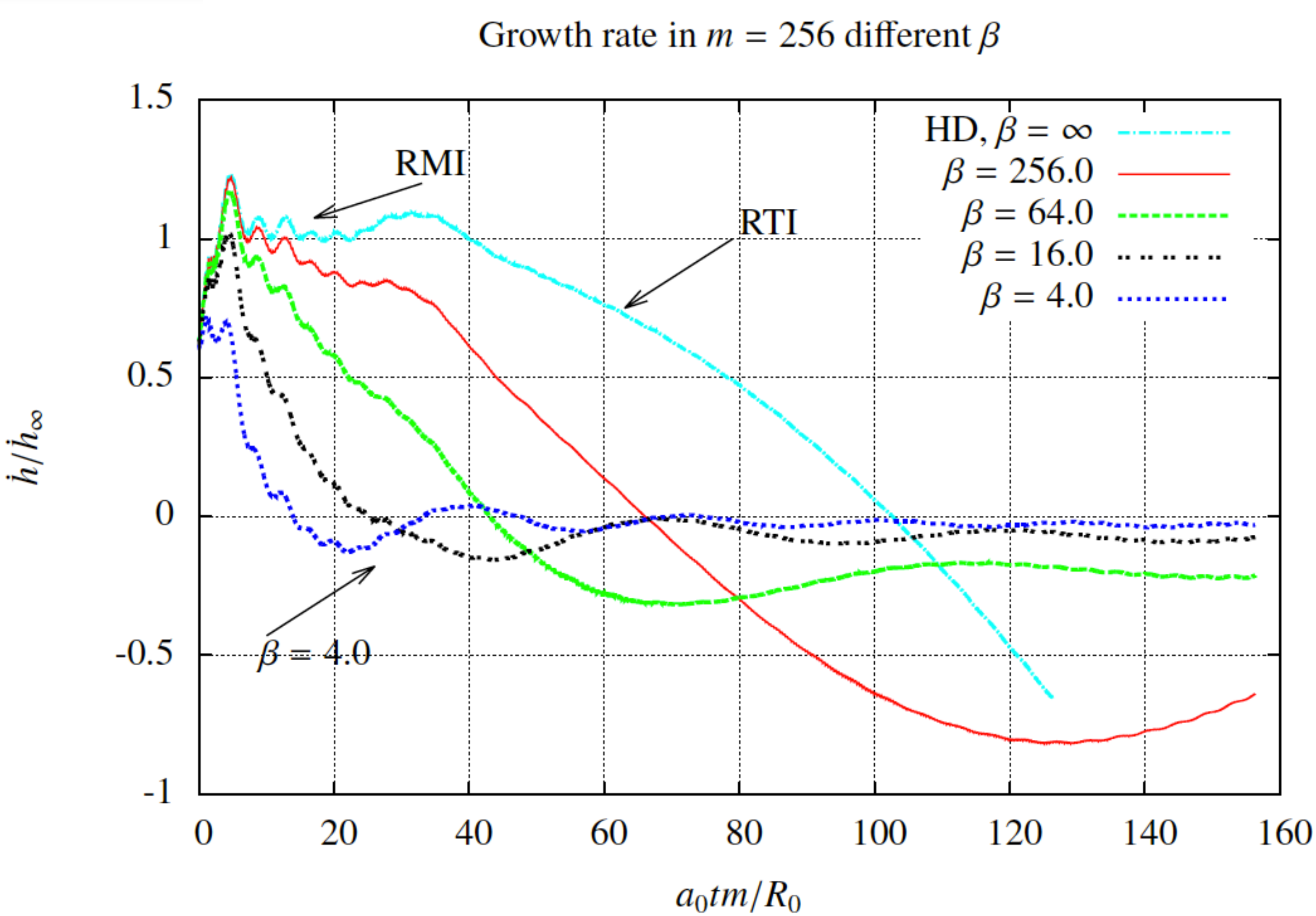
RMI – Transverse Magnetic Field

- Vorticity on the interface breaks up into wave traveling parallel and anti-parallel to the interface
- Interference of these wave causes interface amplitude to oscillate in time
- RMI is still suppressed (Wheatley, Pullin, Samtaney Phys. Fluids 2014)





RMI in Converging Geometry - Linear



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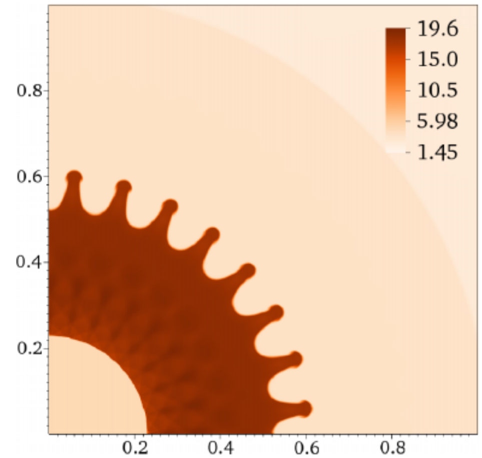
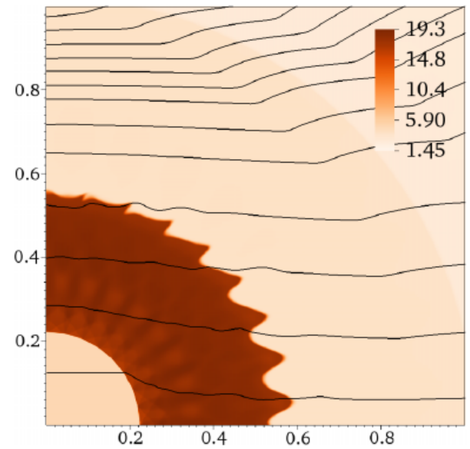
RMI in Converging Geometry - Nonlinear

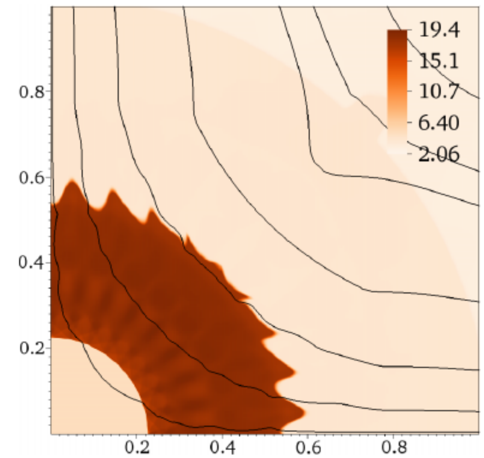
Mostert et al. Phys. Fluids 2015



Axial field

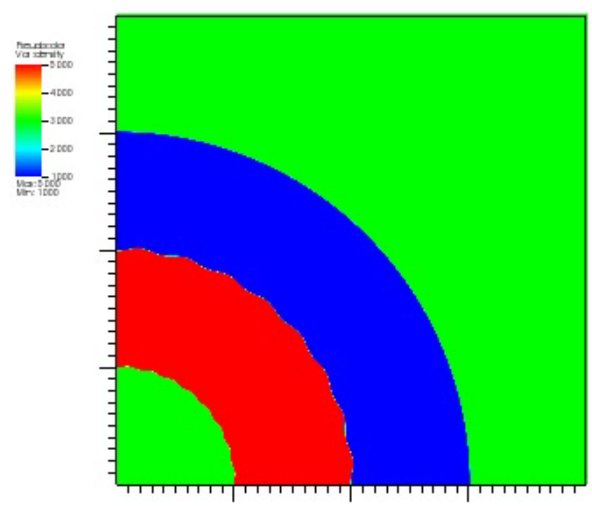


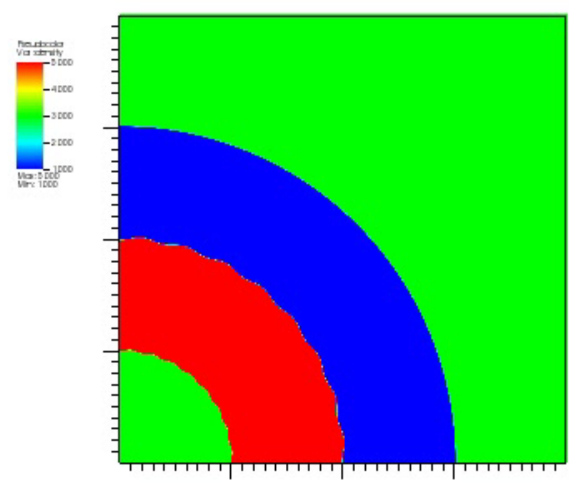
Saddle field



MHD β=32

HD





MHD β=8

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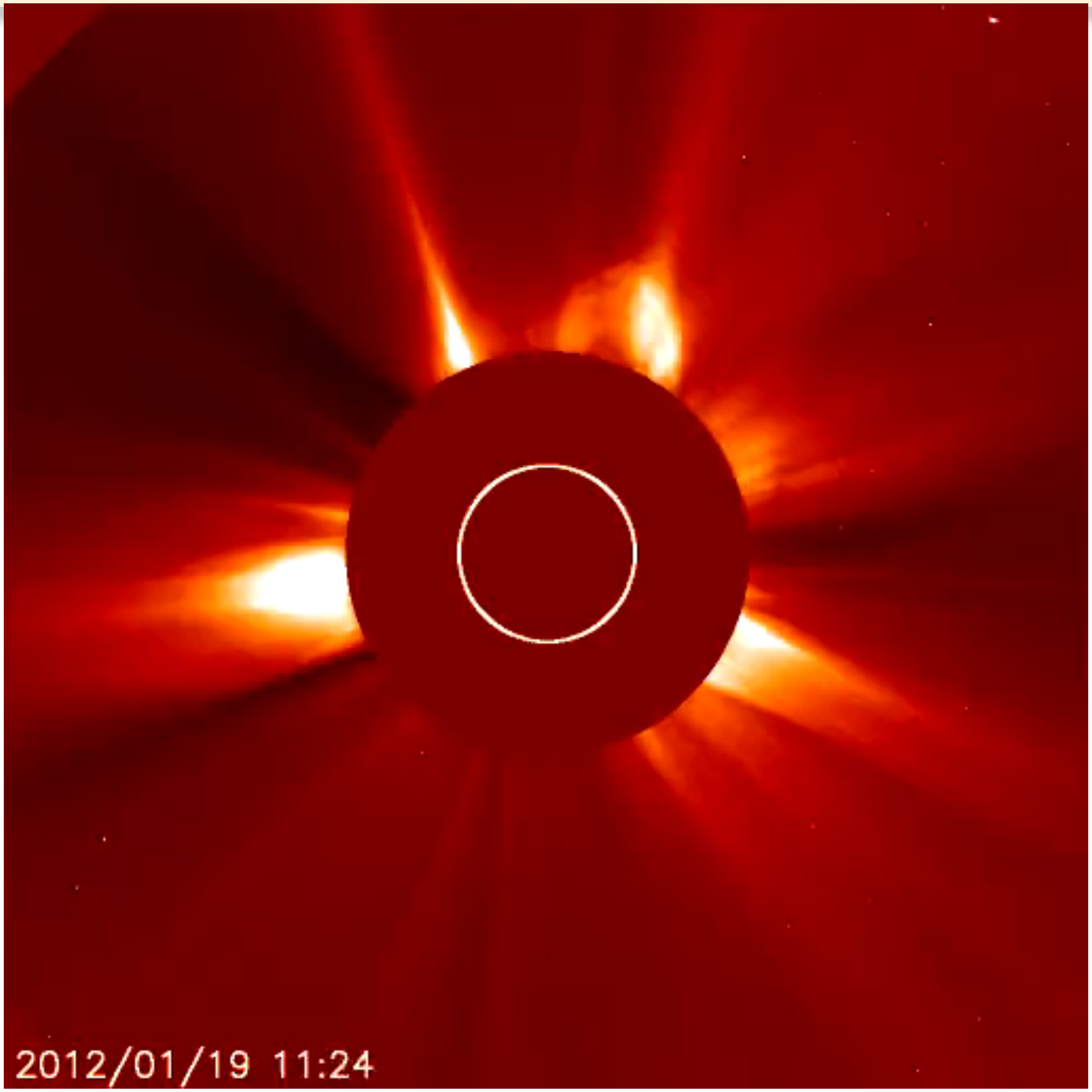
Magnetic Reconnection
Solar Flares (Coronal Mass Ejections)



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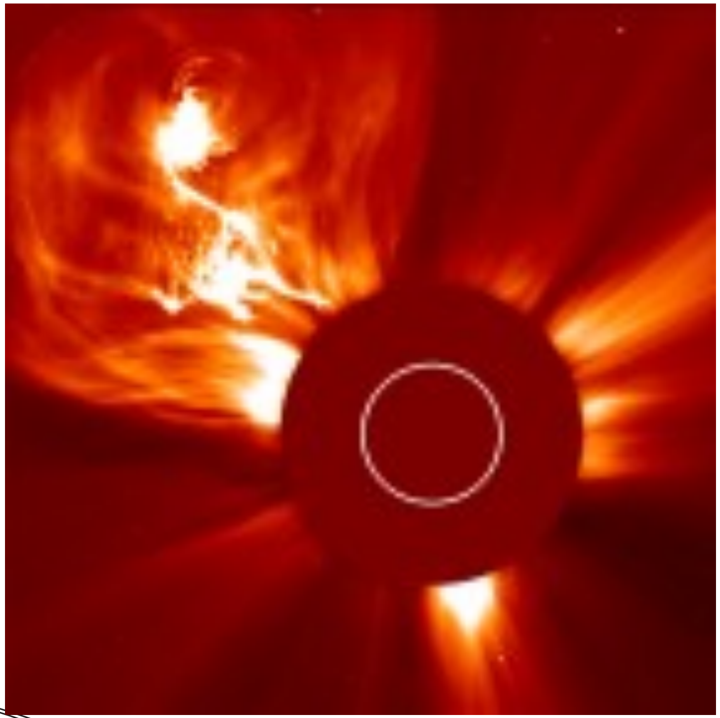
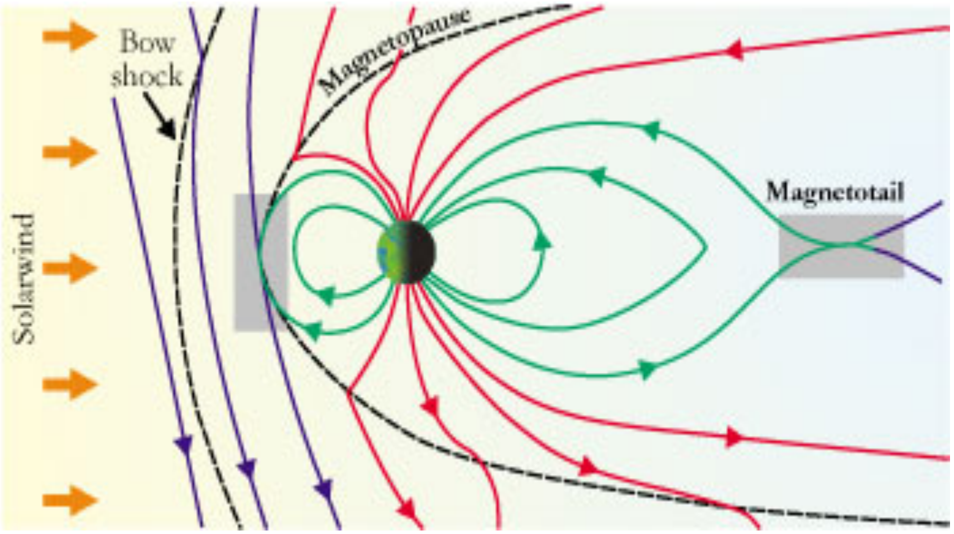
Motivation: solarflares, magnetoshere

Solar flares and Coronal Mass Ejections arise because the magnetic field lines in the Sun break and rejoin in a different configuration.



(taken from: http://sohowww.nascom.nasa.gov/)

Interaction between the solar wind and the earth's magnetic field gives rise to a variety of phenomena, e.g., aurorae

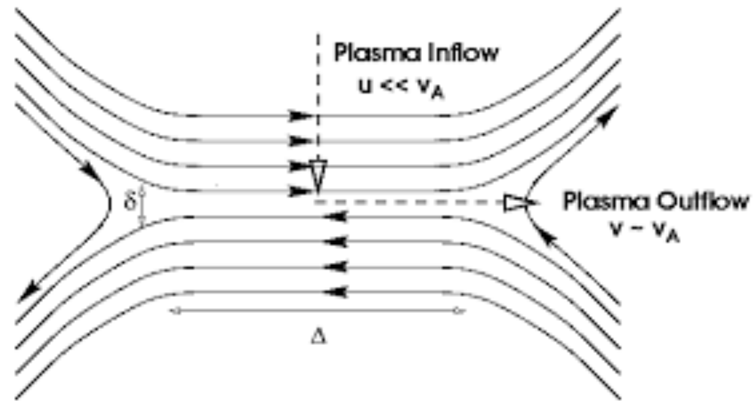


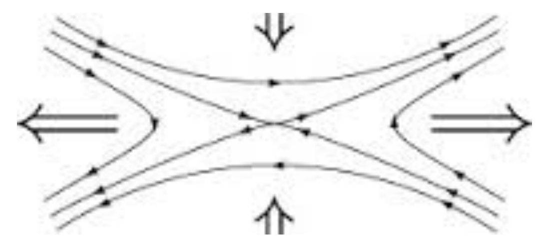
(extracted from: Charles Day, Phys. Today, Oct 2001)

Animation from NASA website

Science Question

- For over 60 years the plasma physics community has struggled with the following question
  - *The explanation of the time scales involved (reconnection in nature is orders of magnitude faster than standard theoretical model aka Sweet-Parker model, 1957-58)*
    - *Example: Solar flare: minutes-hours (nature) and years (model)*
    - *SP model predicts reconnection rate proportional to 1/√S (S, the Lundquist number is the ratio of Alfven wave crossing timescale to resistive diffusion timescale)*





$$S = \frac{\mu_0 L V_A}{\eta}$$

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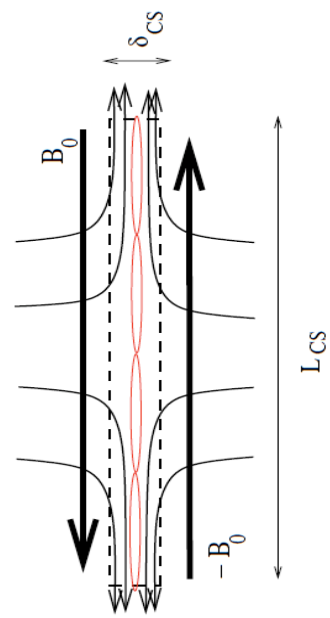
Current sheet instability: threshold

Linear resistive MHD theory (Loureiro et al. PRL 2005) predicts:

$$\gamma_{\max}\tau_A \sim S^{1/4}$$ **Super Alfvénic growth**

$$k_{\max}L_{CS} \sim S^{3/8}$$ **Plasmoids galore**



- For any perturbation to grow, its growth rate needs to exceed the shearing rate:

$$\gamma\tau_A >> 1 \Rightarrow S^{1/4} >> 1$$

→ ***Critical threshold for instability:***

$$S_c \sim 10^4$$

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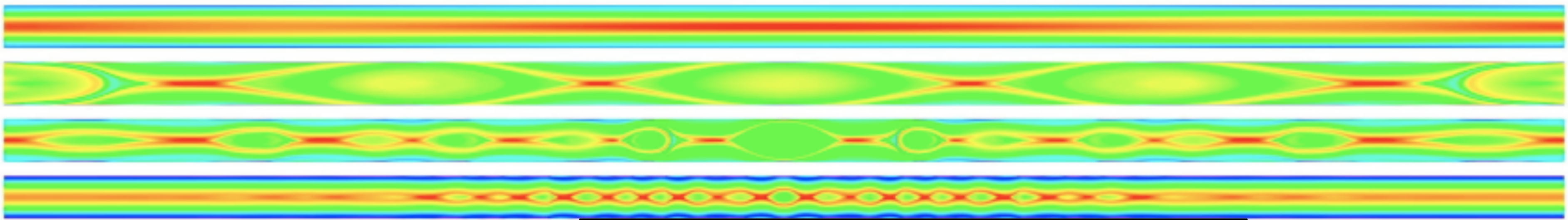
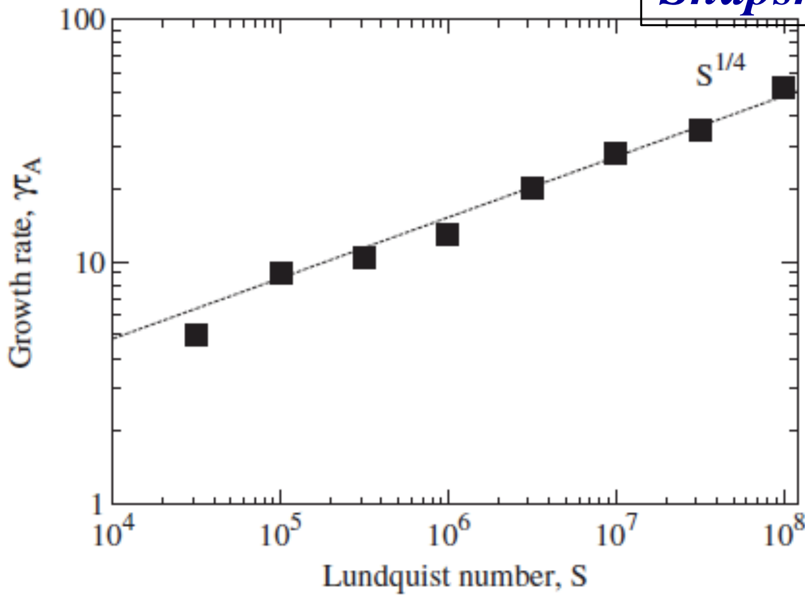
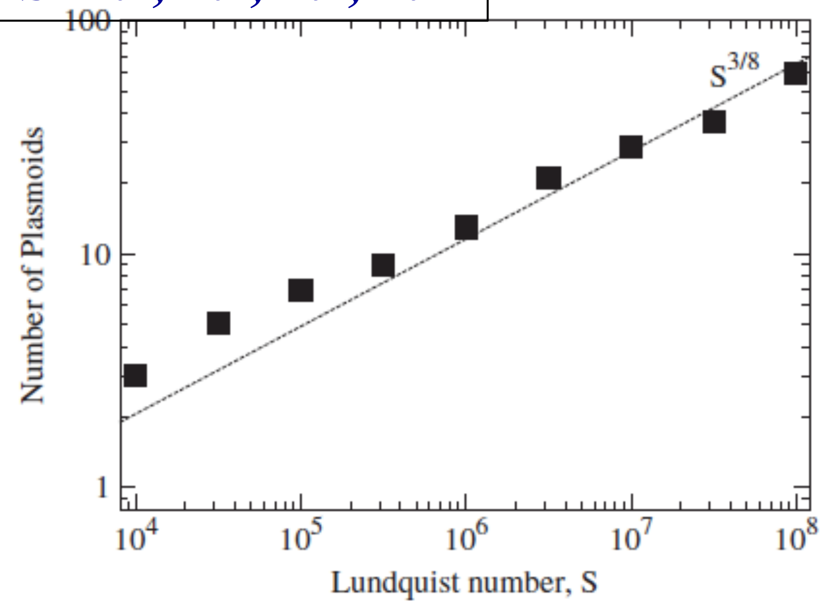
Numerical confirmation of linear theory

Numerical simulations confirm scaling predicted by linear theory (Samtaney *et al*., PRL '09).



Snapshots for S=10^4, 10^5, 10^6, 10^7

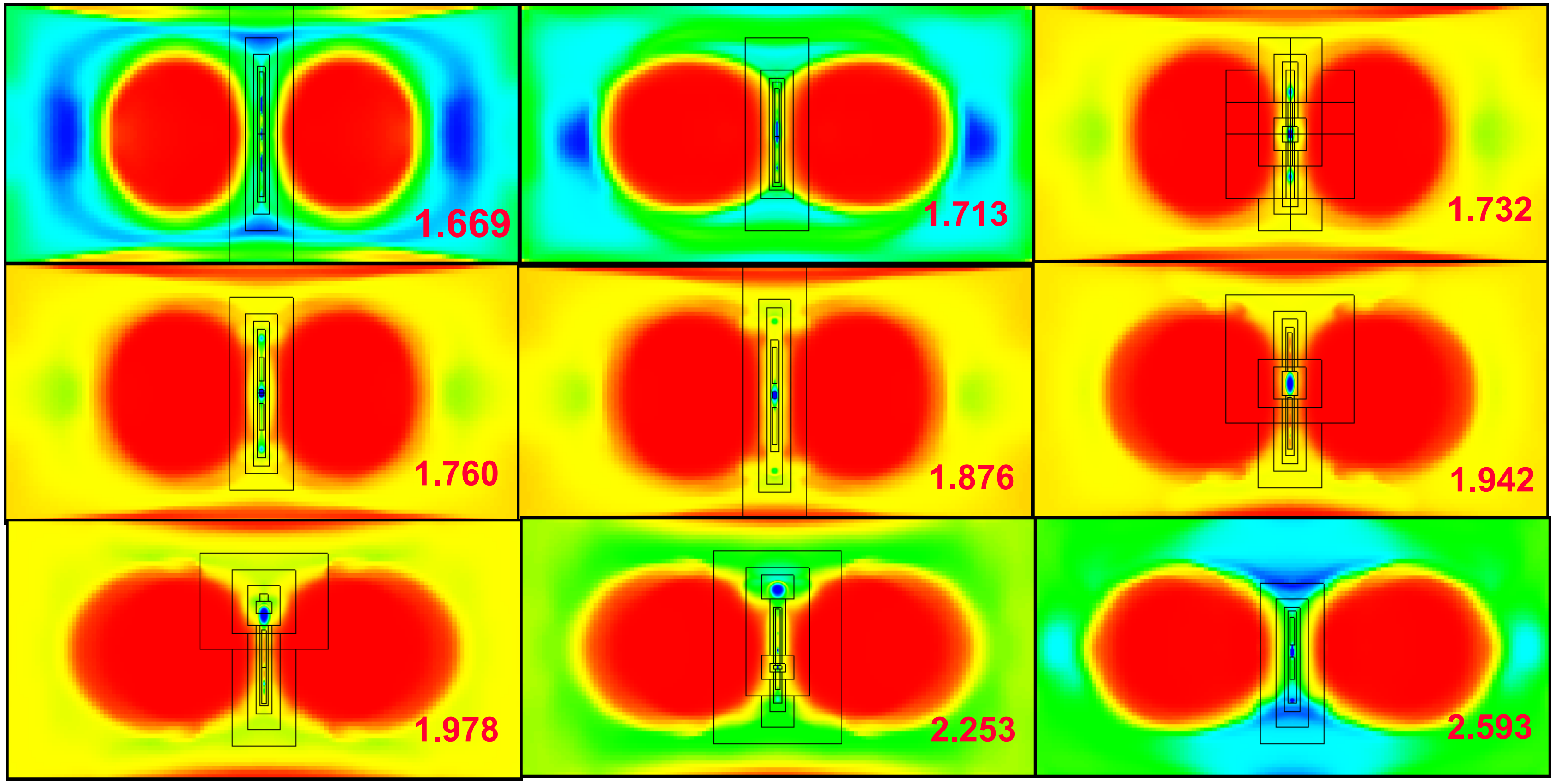




(independently confirmed by Huang et al., PoP '10)

Global Reconnection S= 10^4

High resolution adaptive mesh computations with the AMR-MHD code show plamoid ejections **(Samtaney et al. SciDAC 2005)**



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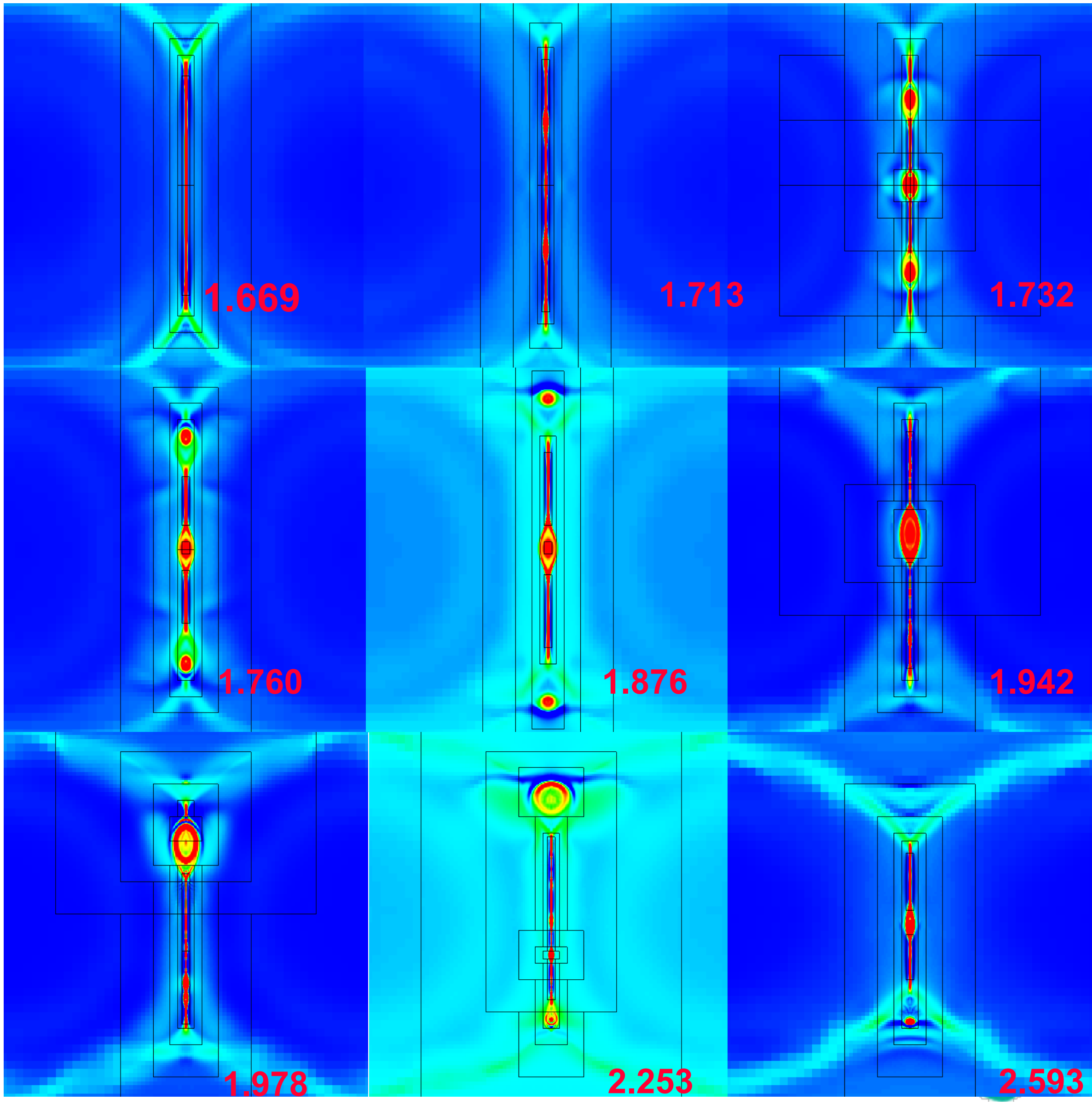
Current: Reconnection S= 10^4

Time sequence of current (J_z)
Thin current layer is unstable and plasmoids form
6 Level AMR run.
Effective unigrid: 4096x2048. **(Samtaney et al 2005)**



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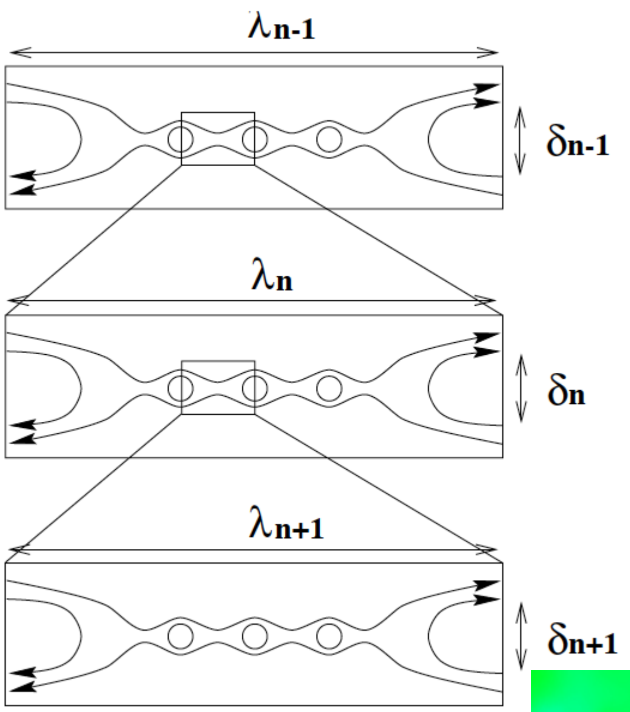
Hierarchical Plasmoid Chains

Long current sheets ($S > S_c \sim 10^4$) are violently unstable to multiple plasmoid formation.



(Shibata-Tanuma '01)

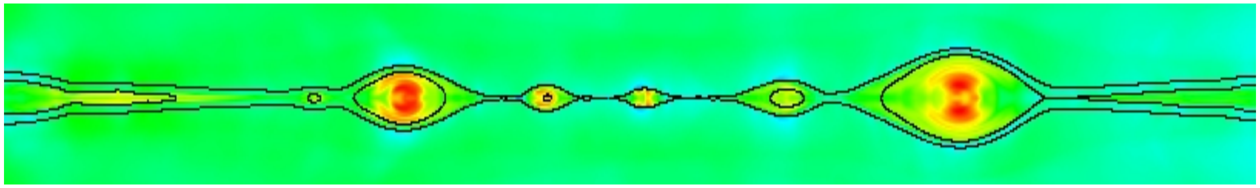
- ***Current layers between any two plasmoids are themselves unstable to the same instability if***

$$S_n = L_n V_A/\eta > S_c$$

- ***Plasmoid hierarchy ends at <u>the critical layer:</u>***

$$L_c = S_c\eta/V_A \quad \delta_c = L_c/\sqrt{S_c}$$

$$cE_c = B_0 V_A/\sqrt{S_c}$$



- ***$N \sim L/L_c$ plasmoids separated by near-critical current sheets.***

Discovery through simulation

Plasmoid-dominated reconnection: the ULS model

Theoretical model (ULS) (Uzdensky et al., PRL '10)

Key results:

- Nonlinear statistical steady state exists; ***effective reconnection rate*** is

  $$E_{eff} \sim S_c^{-1/2} \sim 0.01 \rightarrow \text{ independent of } S$$

- ***Plasmoid flux and size distribution functions*** are:

  $$f(\psi) \sim \psi^{-2} \quad ; \quad f(w_x) \sim w_x^{-2} \quad (\text{because } \psi \sim w_x B_0)$$

- ***Monster*** plasmoids form occasionally:

  $w_{max} \sim 0.1$ L --- can disrupt the chain, observable…

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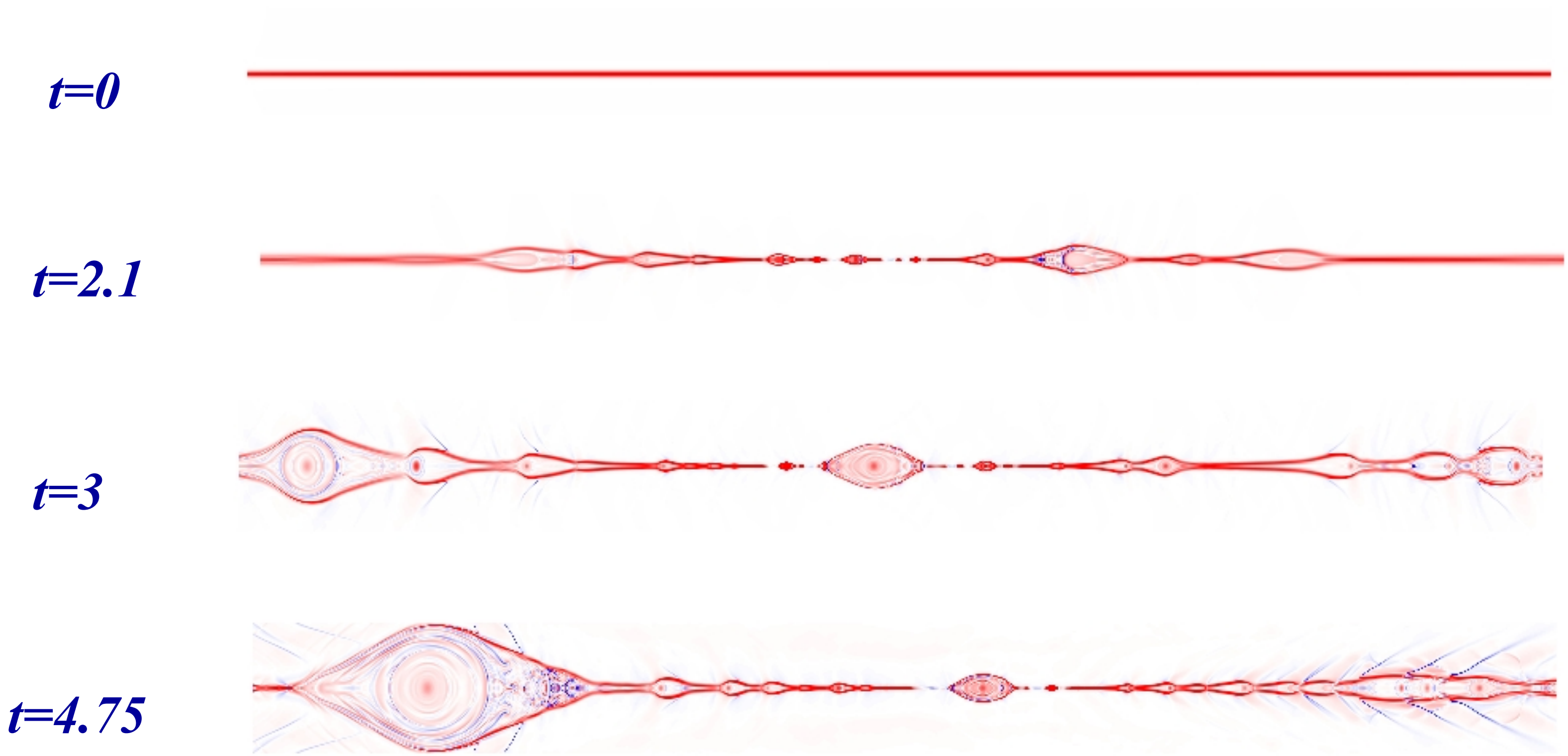
Numerical simulations of CS instability

- Simulations of plasmoid generation and development on Shaheen (IBM Blue Gene, KAUST)



Current sheet evolution, S=10^6

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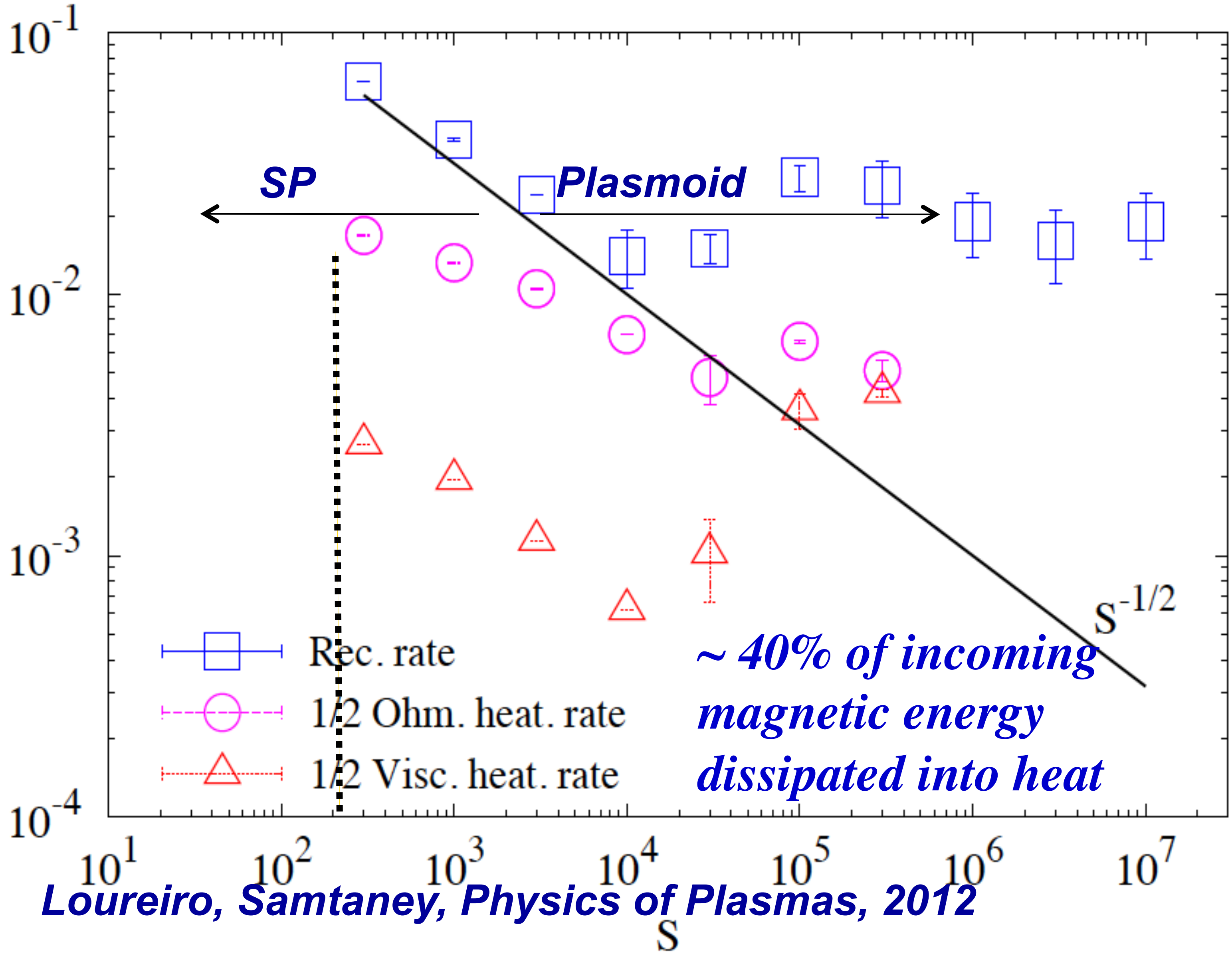
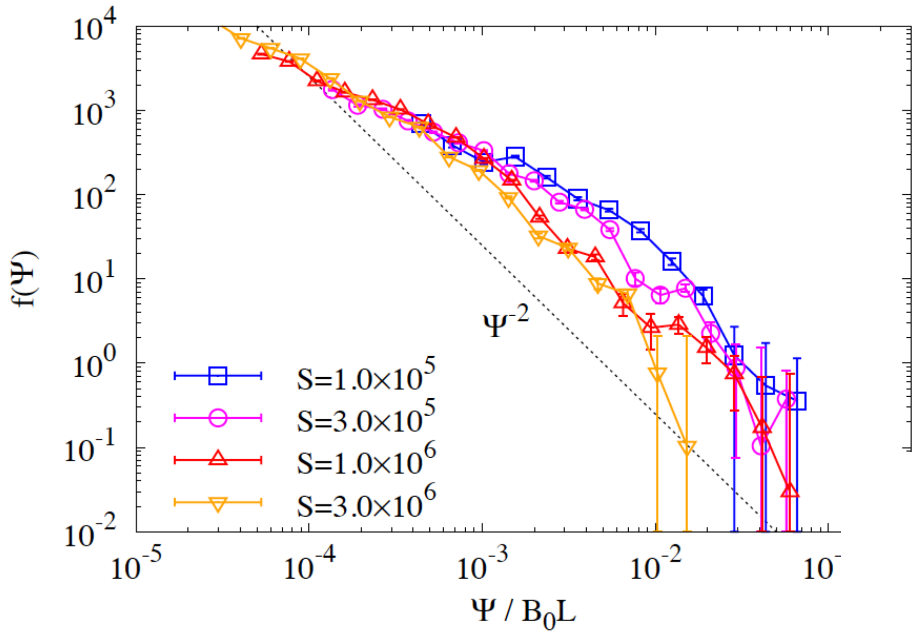
Reconnection and dissipation rates

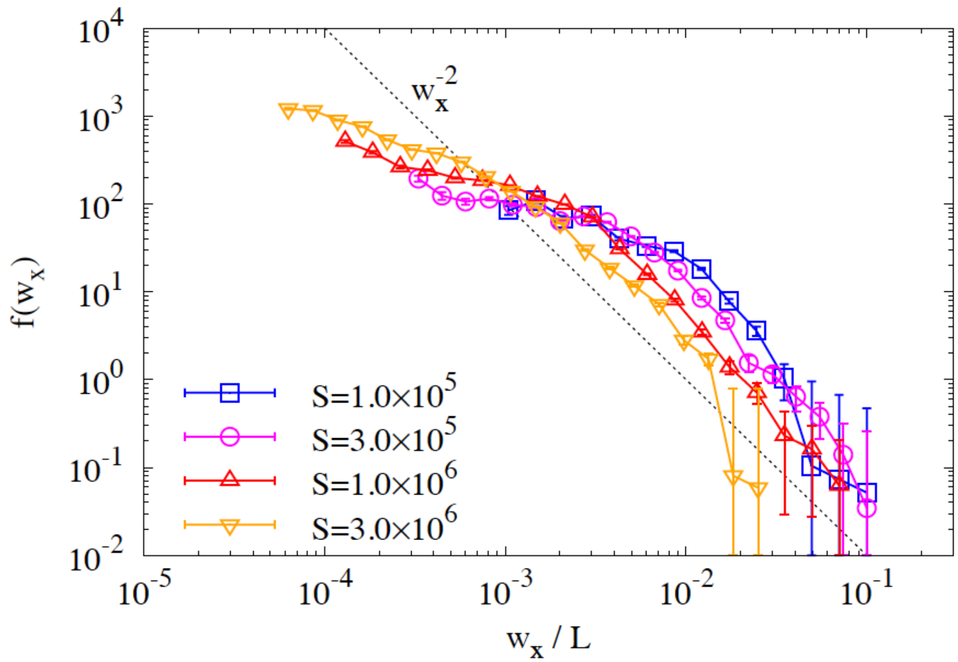


Loureiro, Samtaney, Physics of Plasmas, 2012

Discovery through simulat

Plasmoid width and flux distribution function





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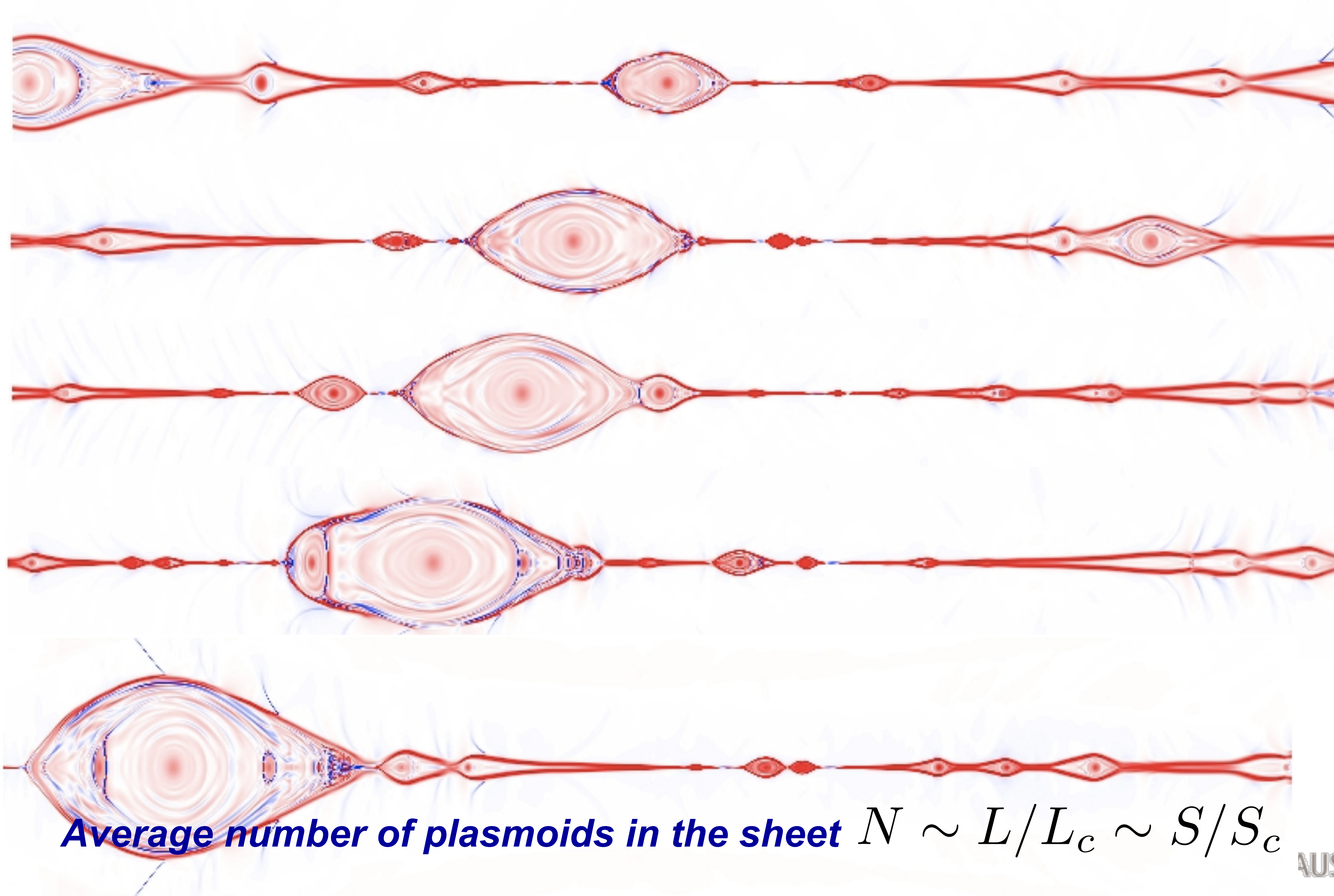
Monster plasmoid formation



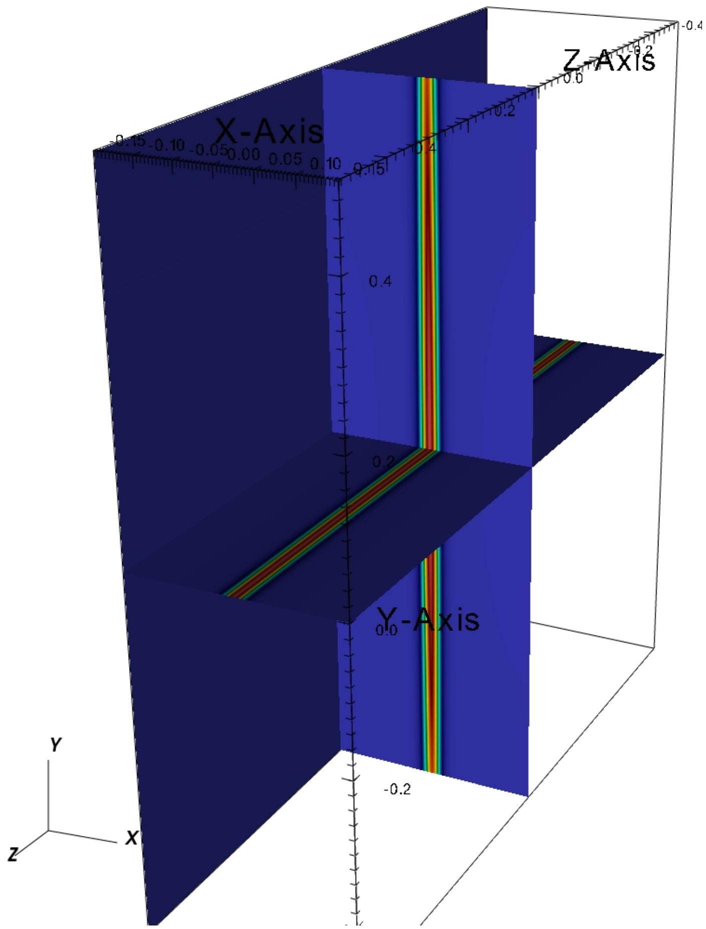
Average number of plasmoids in the sheet $N \sim L/L_c \sim S/S_c$

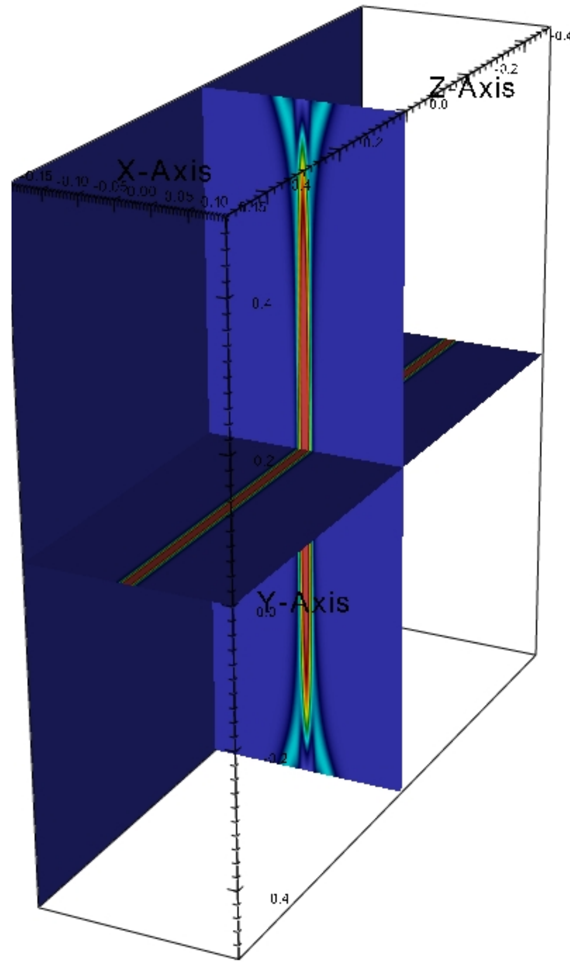
3D Magnetic Reconnection

- Questions remaining for single fluid resistive reconnection
  - *Does the plasmoid enhanced reconnection rate hold in 3D?*
- Nonlinear simulation indicate average number of plasmoids in sheet $N \sim L/L_c \sim S/S_c$
  - *$S=10^6 \sim O(10^2)$ plasmoids ➔ $>O(10^3)$ points along the current sheet*
  - *$S=10^7$ ➔ $\sim O(10^4)$ points. Nearly impossible today?*
- Even with AMR this is an extremely challenging computational problem

Discovery through simulation

Simulation Results: $S=10^4$





t=0

t=7.3

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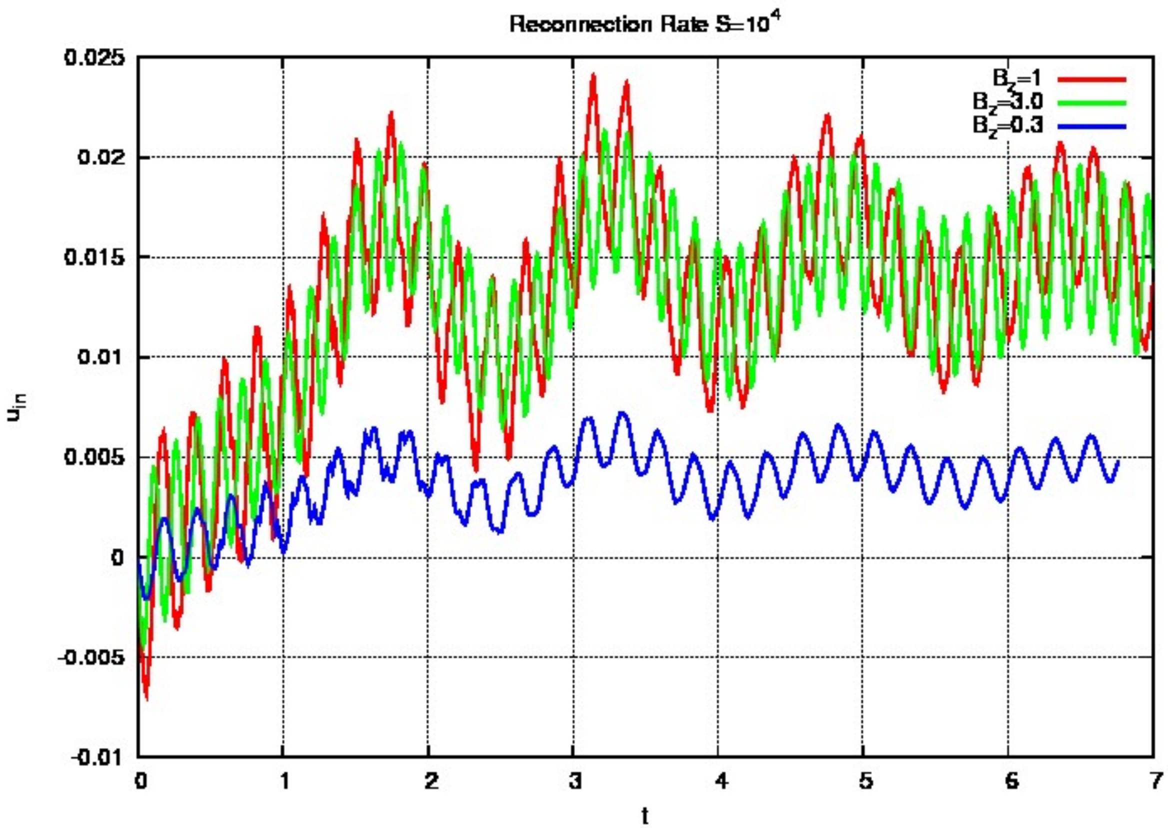
Dependence on B_z



S	B_z	Avg. Recon Rate x 10^2
10^3	0.3	1.55
10^3	1.0	4.93
10^4	0.3	0.47
10^4	1.0	1.43 (≈2D)
10^4	3.0	1.47 (≈2D)

Reconnection rate becomes independent of B_z for large B_z

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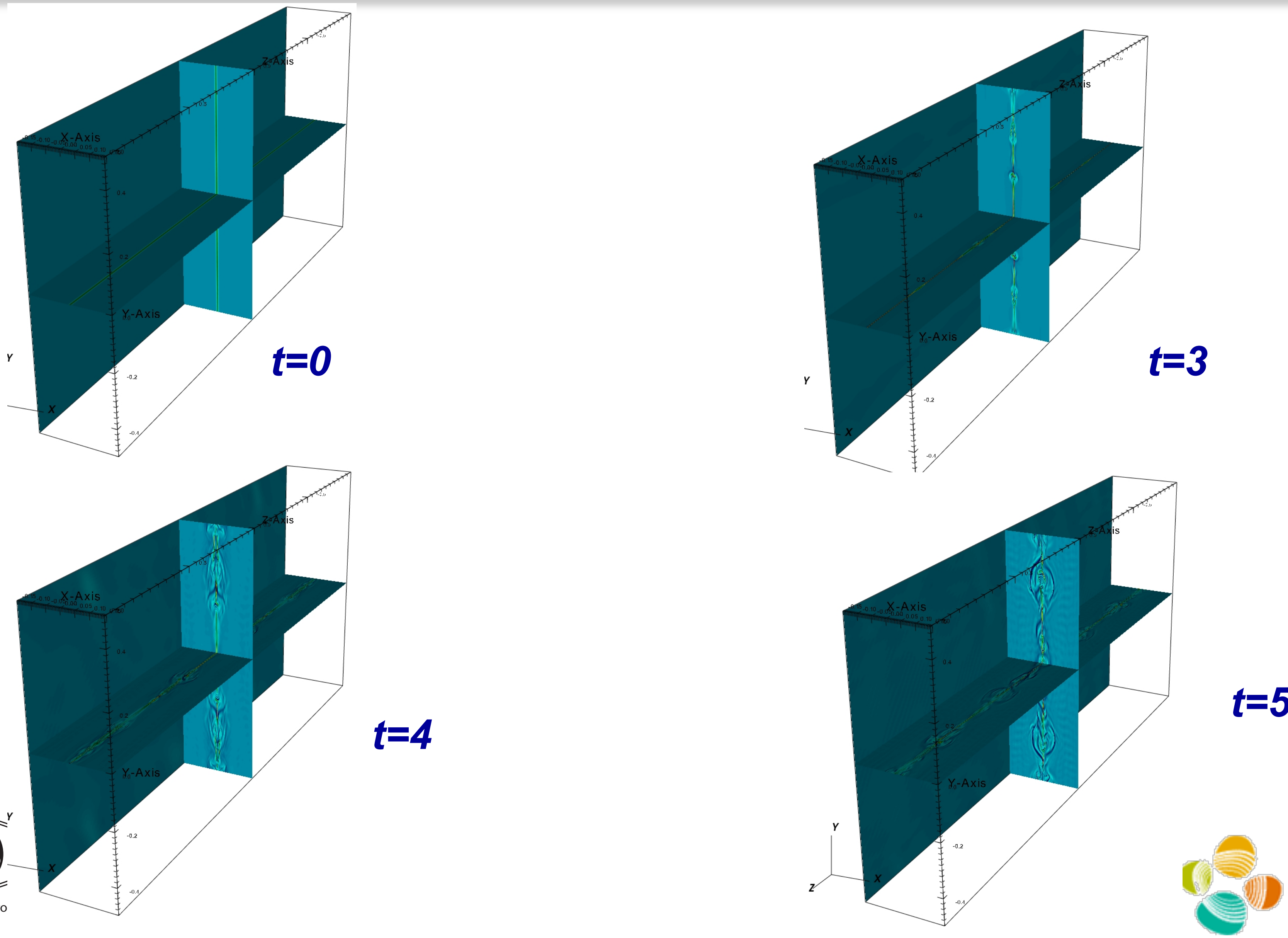
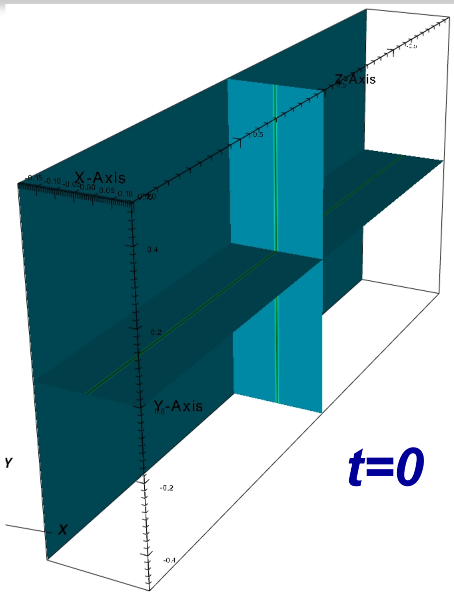
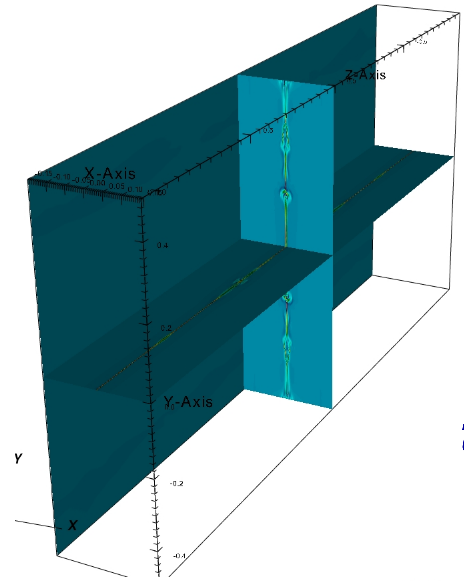
Current Sheet Evolution: $S=10^5$, $B_z=1$



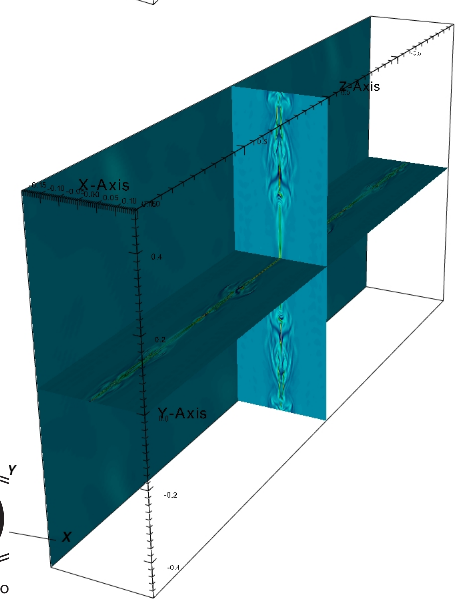
Current Sheet Evolution: $S=10^5$, $B_z=1$



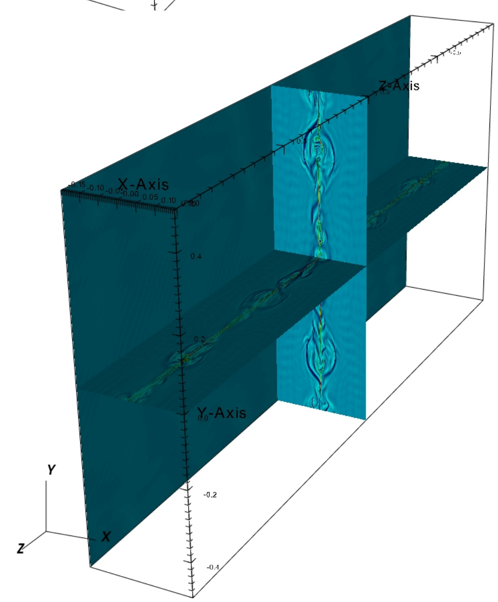
t=0



t=3

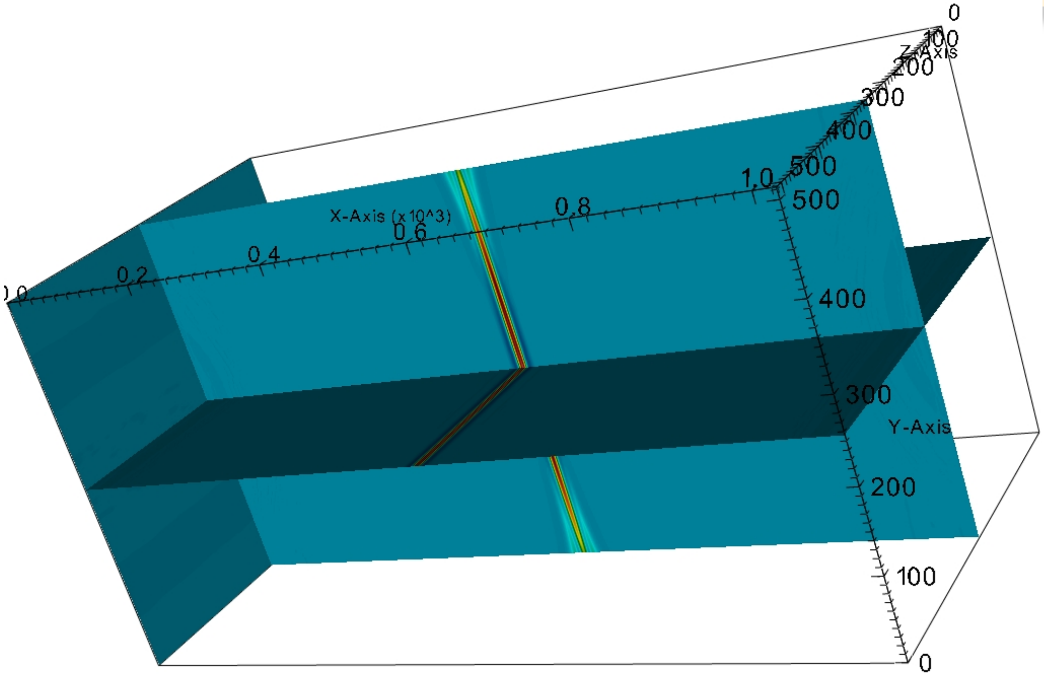


t=4

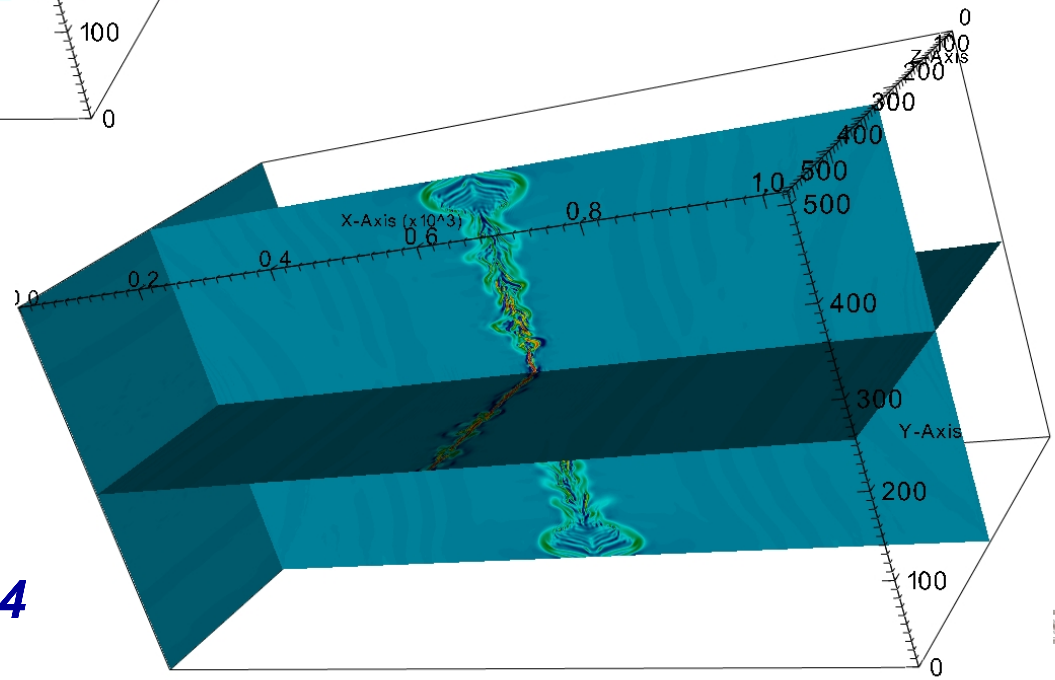


t=5

Current Sheet Evolution: $S=10^6$, $B_z=1$



t=1.2



t=2.4

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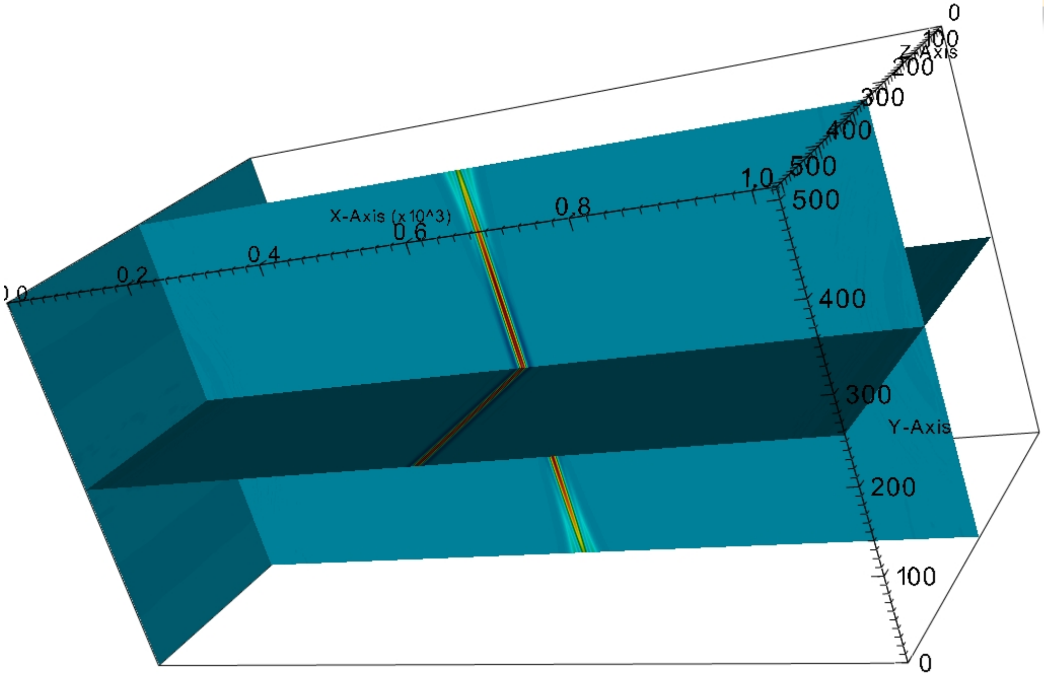
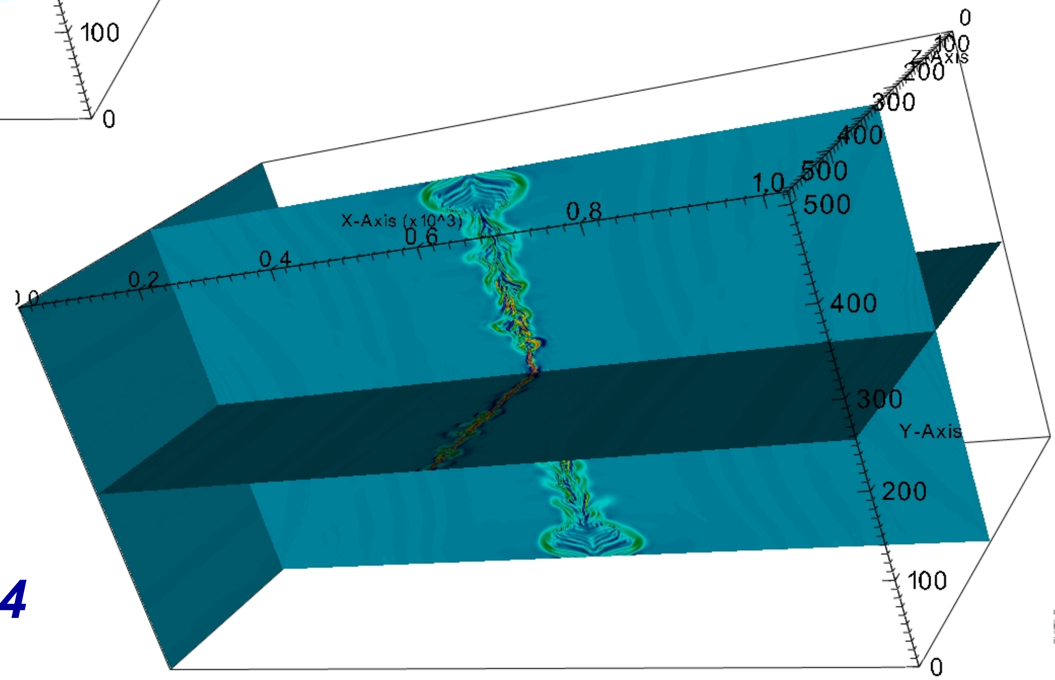
Current Sheet Evolution: $S=10^{6}$, $B_z=1$



t=1.2



t=2.4

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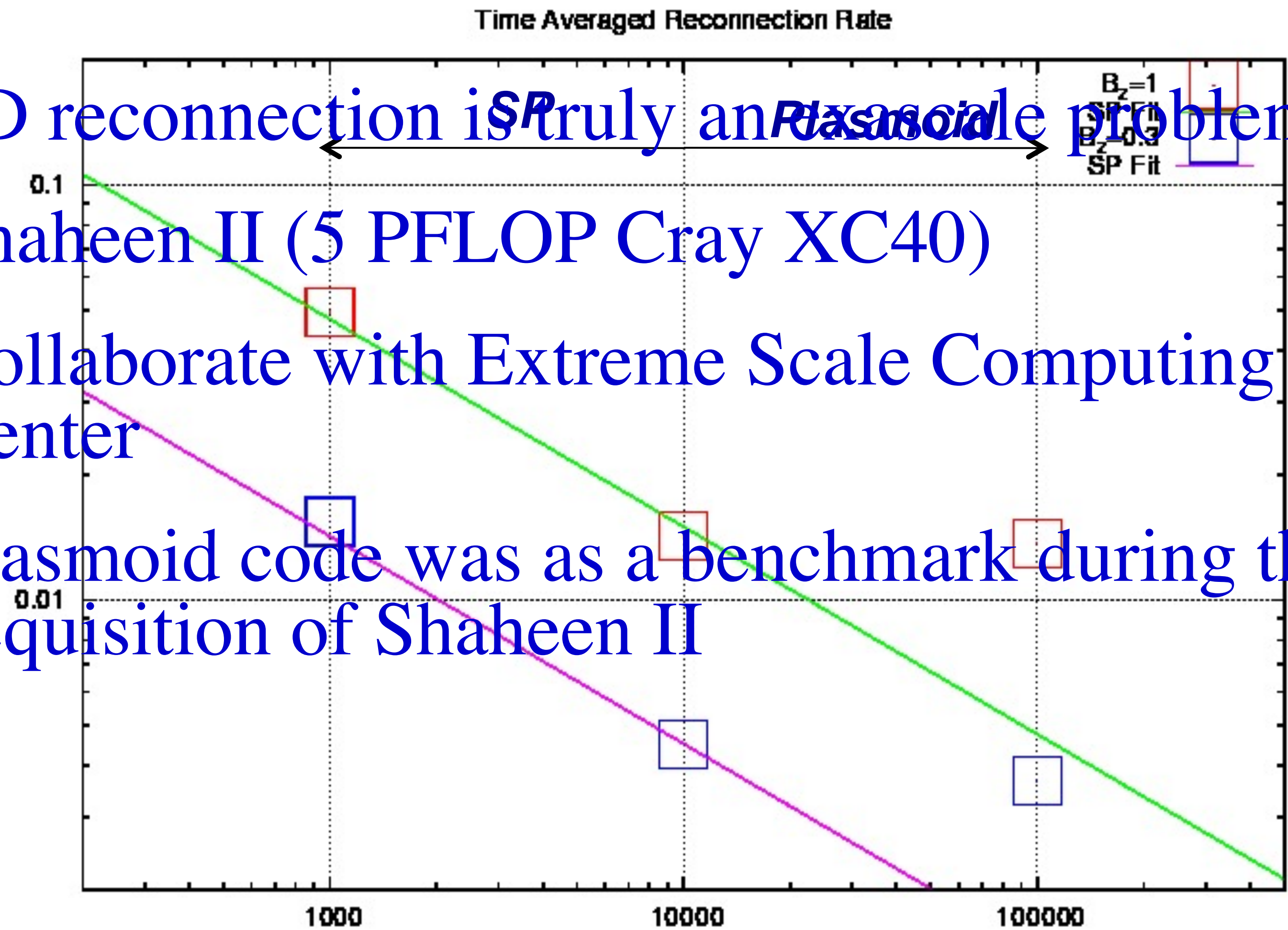
Time Averaged Reconnection Rate



- 3D reconnection is truly an exascale problem
- Shaheen II (5 PFLOP Cray XC40)
- Collaborate with Extreme Scale Computing Center
- Plasmoid code was as a benchmark during the acquisition of Shaheen II

Discovery through simulation

Wall Bounded Turbulence

- Applications Driver: Computing wall-bounded turbulent flows is extremely challenging. Most engineering applications of turbulent flows are of the wall-bounded variety
  - *Holy grail: computing flow over a sphere to reproduce the drag crisis (Re~ 300,000)*
  - *DNS: $Re^{9/4}$*
  - *TBL DNS: $Re^{37/14}$*
  - *TBL WR LES: $Re^{13/7}$*

- Research: Development of wall models and high-fidelity simulation codes for wall-bounded turbulent flows and applying these to flows over bluff bodies wind turbines components (e.g. airfoils) and wind farms (KAUST + Caltech collaboration)

- Key physics issues: separation, adverse pressure gradients, curvature

Strong correlation of maxima of Reynolds stress with displacement thickness is observed in experiments

(Zhang & Samtaney, Computers & Fluids, 2015)

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Inner wall scaling laws

- <u>Question</u>: Does the velocity profile in a wall-bounded turbulent flow obey a log-law or a power-law scaling?
  - *Controversy ongoing for over two decades*
- Log law
  - *The law of the wall, by Prandtl (1932)*
  - *The defect law, by von Kármán (1930)*
  - *Matching procedure, by Millikan (1938)*

$$U^+ = \frac{1}{k}\log z^+ + B$$

- Power law
  - *Barenblatt, Chorin and Prostokishin (BCP law)*
    - *JFM 1993, PNAS1997, PNAS2000, JFM2000*
  - *George and Castillo (GC law)*
    - *Appl. Mech. Rev. 1997, AIAA J. 2006*
      - *Power law for TBL,*
      - *log law for Channel and pipe*

$$U^+ = C(z^+ + a)^\gamma$$

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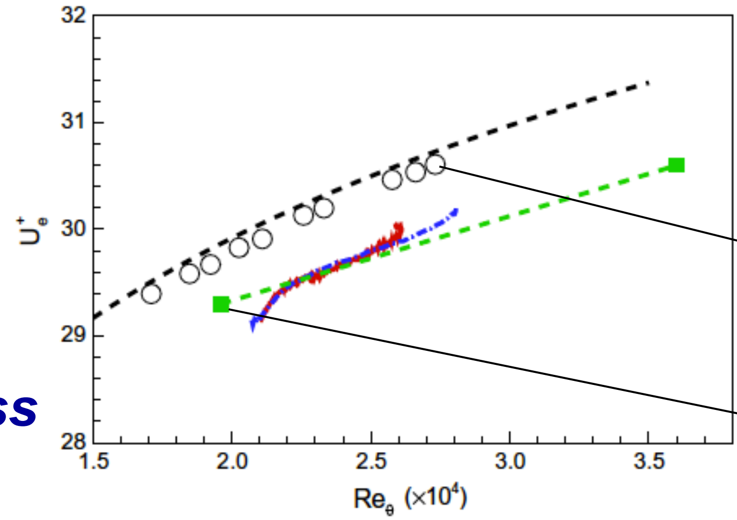
Log Law or Power Law?

- Developed a turbulent boundary layer (TBL) large-eddy simulation code
- Systematically i … els: each intrinsically employs the log
- Large scale sim … ds numbers on Shaheen

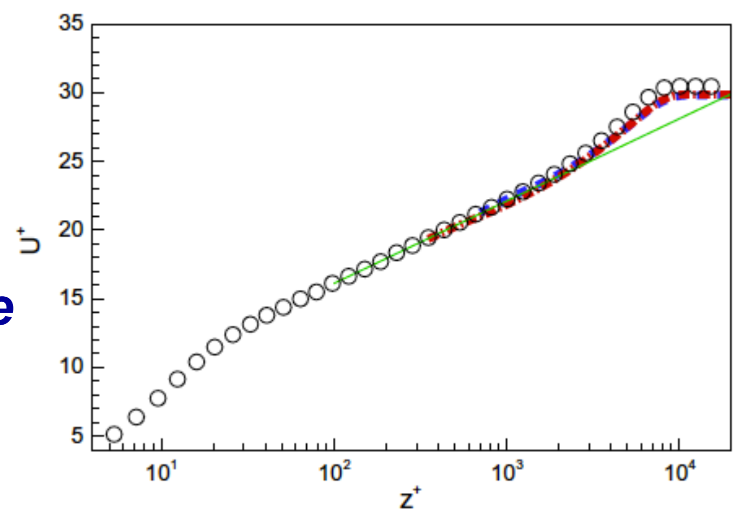
Wall shear stress



Osterlund, 1999

Mathis et al. 2011

Mean vel. profile



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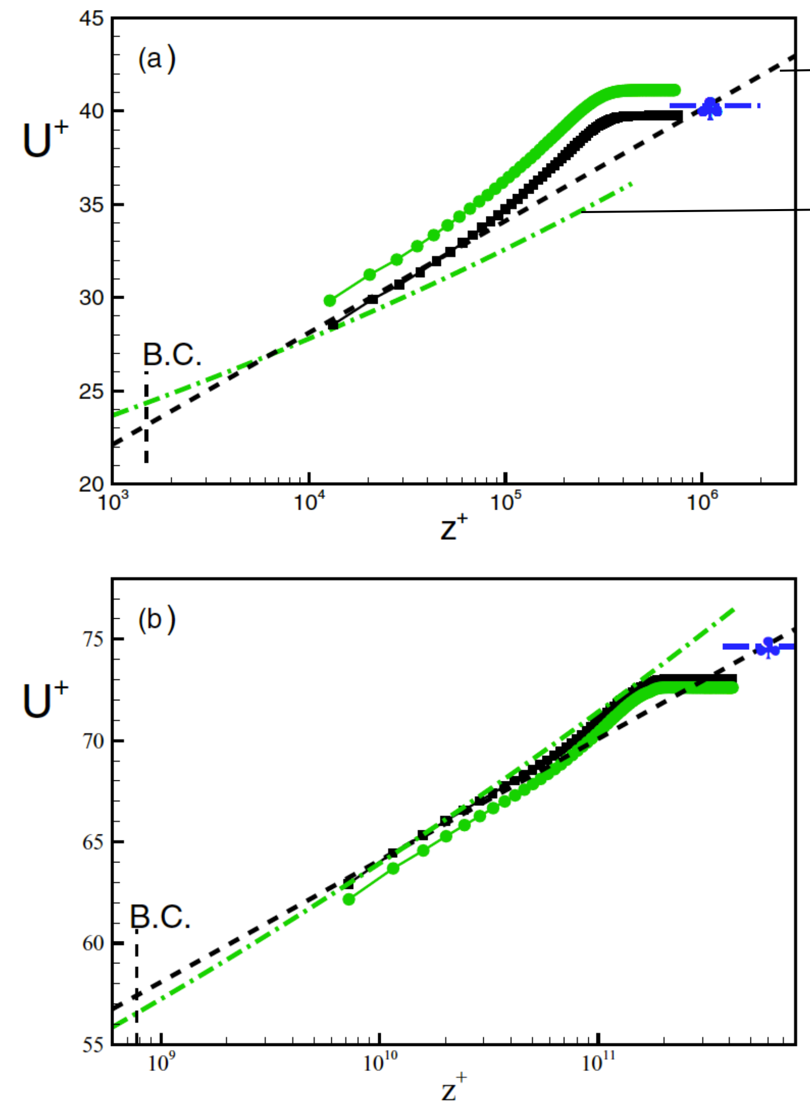
Log Law or Power Law?



Log-law fit

Power-law fit

$Re_\theta \sim 10^6$

$Re_\theta \sim 10^{11}$

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Log Law or Power Law?

Relative difference between computed and theoretical velocity gradient

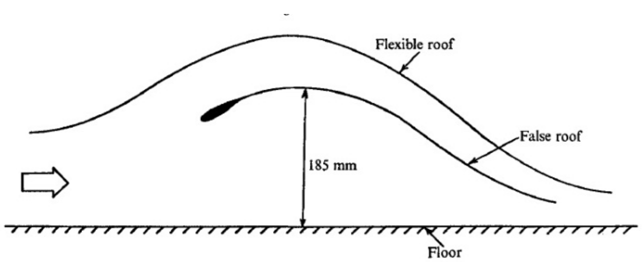
	Re_θ	Log-law	GC-law
LES-L	1.4×10^4	18%	20%
	1.2×10^5	14%	26%
	1.0×10^6	11%	24%
	9.2×10^6	9.6%	20%
	8.1×10^7	8.1%	15%
	7.8×10^8	7.0%	6.6%
	7.2×10^9	5.3%	5.4%
	6.9×10^{10}	4.6%	13%
	6.6×10^{11}	2.8%	20%
LES-P	1.3×10^4	12%	34%
	1.1×10^5	10%	70%
	1.0×10^6	6.8%	50%
	9.0×10^6	4.7%	23%
	8.2×10^7	3.2%	9.1%
	7.6×10^8	3.7%	1.7%
	7.3×10^9	2.5%	3.8%
	6.8×10^{10}	2.3%	13%
	6.7×10^{11}	0.63%	21%

Monotonic decrease

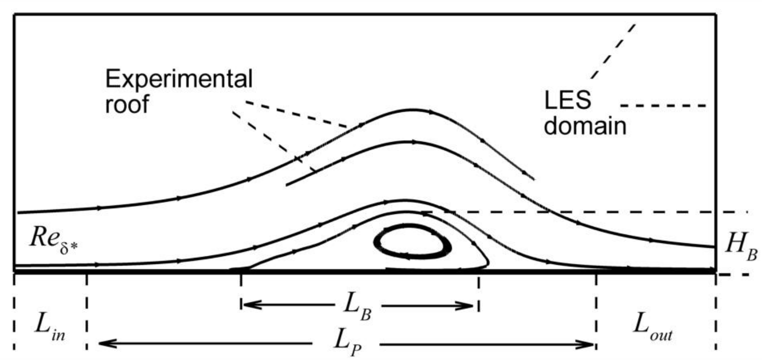
Turbulent separation/reattachment bubble

- DNS:
  - *Na & Moin (1998), Skote & Henningson (2002)*
- Experiments
  - *Perry & Fairlie (1975), Patrick (1987), …, Lögdberg (2006)*

Experiment



LES



- ***Presently:***
  - ***Use parallelepiped (rectangular domain)***
  - ***Replace upper wall by a stream-wise distribution of wall-normal velocity***
  - ***Match wall pressure distribution to experiments***

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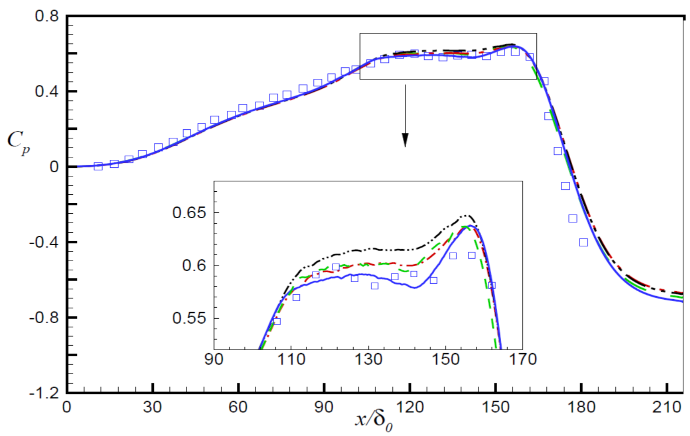
TBL With Separation

Perry and Fairlie (1975); Re_θ =2,000



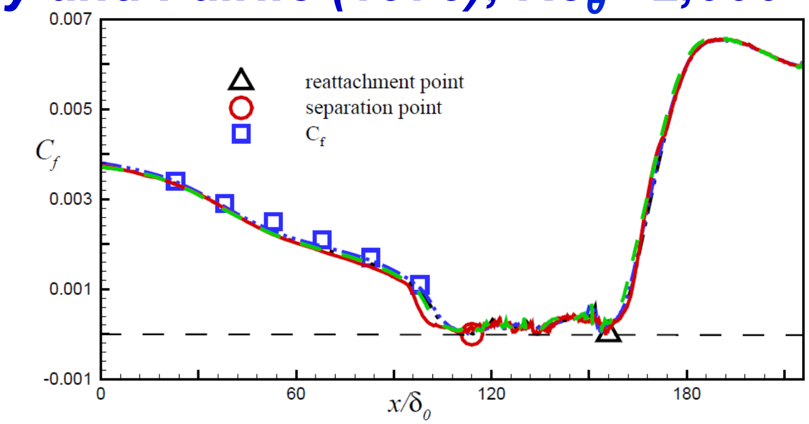
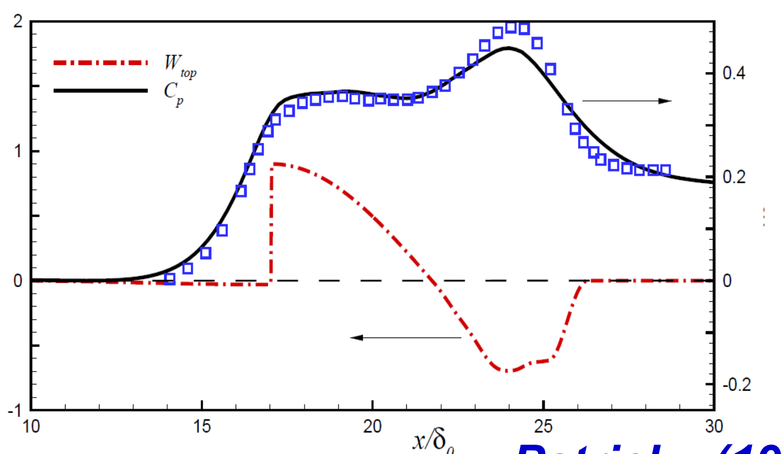


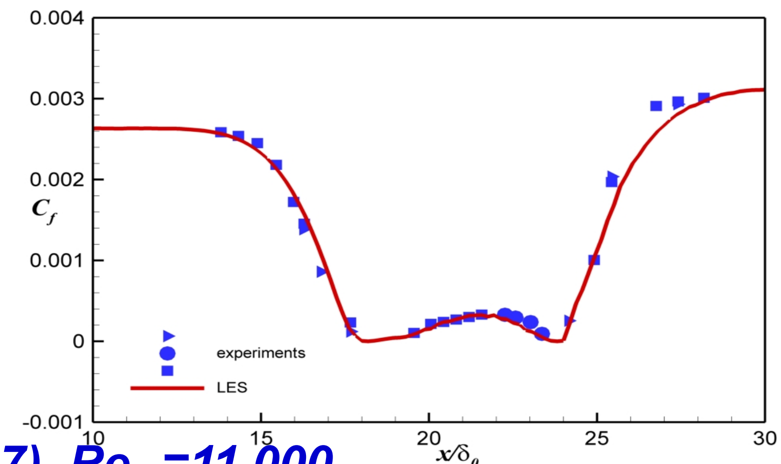
FIGURE 8. Skin friction coefficient C_f. Symbols for experiments by Perry & Fairlie (1975), lines for present LES. □ , C_f; ○ , separation point; △ , re-attachment point; – – – – , case $C0$; —·— , case $C1$; —··— , case $C2$; ——— , case $F1$. Horizontal dashed line indicates $C_f = 0$.

□ ***Experiment (Perry & Fairlie, 1975)***

LES (different resolution))

Cheng et al. JFM 2015





Patrick (1987), Re_θ =11,000

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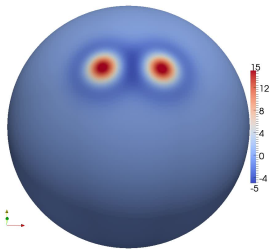
Conclusion

- RMI is suppressed by a magnetic field
  - *Baroclinically generated vorticity is transported away by MHD shocks (nonlinear) or Alfvén fronts (linear)*
- Magnetic reconnection
  - *Plasmoid dominated instability of current sheet*
  - *Reconnection rate saturates for $S>10^4$*
- Turbulent boundary layers on a flat plate
  - *With increasing Re, the log-law fit is better than power-law*
- In all three cases large-scale simulations were the means driving the discovery

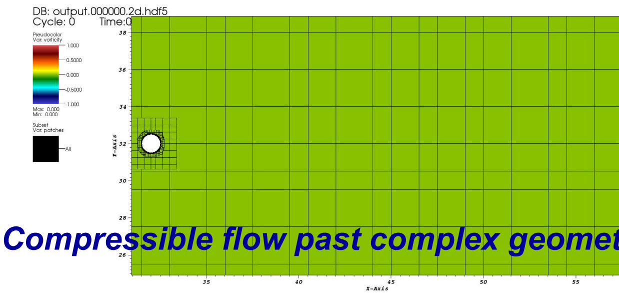
Other ongoing investigations

CFD using discrete exterior calculus
Mamdouh Mohamed



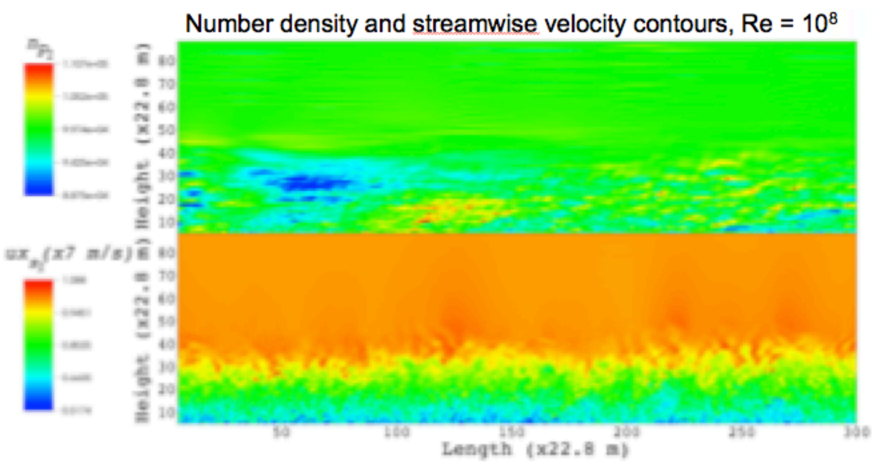
Taylor vortices over sphere

Embedded boundary + AMR
Mohamad Al-Marouf



Compressible flow past complex geometries

DNS/LES modeling
Wei Zhang, Wei Gao, Mustafa Rahman



Effect of contraction on turbulence
Ram Ramakrishnan, Sriram Rengarajan, Siggurgur Thoroddssen

Similarity solutions in MHD
Chris Moore

Non-model Stability of Vlasov Plasma
Valeria Ratushnaya

High-order methods for MHD
Yuan Li

Stability analysis of droplets
Junaid Siddiqui

Fluctuating nano-scale hydrodynamics
Kiran Narayanan

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- RMI
  - *Prof. Dale Pullin (Caltech), Dr. Vince Wheatley (UQ)*
  - *US DOE, ARC, KAUST CRG*
- MR
  - *Dr. Nuno Loureiro (IPFN Portugal) Prof. Alex Scheckochihin (Oxford), Prof. Dmitry Uzdensky (Colorado)*
  - *US DOE, KAUST Baseline*
- TBL
  - *Prof. Dale Pullin (Caltech), Dr. Wan Cheng (Caltech), Wei Zhang (KAUST)*
  - *KAUST CRG*

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Thank You!

"BUT THIS IS THE SIMPLIFIED VERSION FOR THE GENERAL PUBLIC."